9th Solid Chemistry Conference

SCC 2023

Organized by the

Tunisian Chemical Society

17-20 December 2023

Barceló Concorde Green Park Palace Hotel
El Kantaoui-Sousse, Tunisia

Abstracts of Lectures and Communications
List of Participants

Tunisian Chemical Society - Short Program of SCC 2023

SUNDAY 17 DECEMBER 2023	
14.00 – 17.00	**Welcoming participants, distribution of documents and check in**
17.00 – 17.30	**Opening Ceremony**
17.50 – 18.30	**Lecture 1** **Kishor Kumar SADASIVUNI** - *Introduced by* Adel MEGRICHE *Center for Advanced Materials, Qatar University, Doha, Qatar*
MONDAY 18 DECEMBER 2023 (Morning)	
09.00 – 09.40	**Lecture 2** **Rezan DEMIR-CAKAN** - *Introduced by* Mohamed Lotfi EFRIT *Chemical Engineering, Gebze Technical University, Kocaeli, Türkiye*
09.40 – 10.20	**Lecture 3** **Mohamed BOUOUDINA** - *Introduced by* Mehrez ROMDHANE *Energy, Water, and Environment Research Lab, Prince Sultan University, Riyadh, Saudi Arabia*
10.20 – 10.40	**Gathering for the group photo**
10.40 – 11.15	**Poster Session 1 (P 01 - P 30) Alphabetical Order**
11.15 – 12.30	**Oral Communications - Session 1 : OC 01 - OC 05**
13.00	**Lunch**
MONDAY 18 DECEMBER 2023 (Afternoon)	
15.00 – 15.40	**Lecture 4** **Deepalekshmi PONNAMMA** - *Introduced by* Latifa BERGAOUI *Research Quality Section, Research Planning and Development Department, Qatar University, Doha, Qatar*
15.45 – 17.00	**Oral Communications - Session 2 : OC 06 - OC 10**
17.00 – 17.45	**Coffee Break & Poster Session 2 (P 31 - P 62) Alphabetical Order**
17.45 – 19.00	**Oral Communications - Session 3 : OC 11 - OC 15**
19.00	**Dinner**
TUESDAY 19 DECEMBER 2023 (Morning)	
09.00 – 09.40	**Lecture 5** **Roohollah BAGHERZADEH** - *Introduced by* Latifa LATROUS *Institute for Advanced Textile Materials and Technologies, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran*
09.40 – 10.20	**Lecture 6** **Shahzada AHMAD** - *Introduced by* Mohamed DAMMAK *BCMaterials, Basque Center for Materials, applications & Nanostructures, University of Basque Country Science Park, Leioa, Spain*
10.20 – 11.00	**Poster Session 3 (P 63 - P 94) Alphabetical Order**
11.00 – 12.30	**Oral Communications - Session 4 : OC 16 - OC 21**
13.00	**Lunch**
TUESDAY 19 DECEMBER 2023 (Afternoon)	
15.00 – 16.30	**Oral Communications - Session 5 : OC 22 - OC 27**
16.30 – 17.15	**Coffee Break & Poster Session 4 (P 95 - P 127) Alphabetical Order**
17.15 – 18.45	**Oral Communications - Session 6 : OC 28 - OC 33**
19.00	**Dinner**
WEDNESDAY 20 DECEMBER 2023	
09.00 – 09.40	**Lecture 7** **Mohamed ABDEL SALAM** - *Introduced by* Béchir CHAOUACHI *Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia*
09.45 – 10.45	**Oral Communications - Session 7 : OC 34 - OC 37**
11.00 – 12.00	**Oral Communications - Session 8 : OC 38 - OC 41**
12.00	**Closing Remarks and Poster Awards**
13.00	**Lunch, Check Out and Departure**

FOREWORD

On behalf of the Tunisian Chemical Society (TCS), we would like to extend our warmest welcome to the entire scientific community working in the field of Solid State Chemistry, both in national and international spheres, who have accepted to participate in the 9th Solid Chemistry Conference (SCC 2023), which is held from 17 to 20 December 2023, in the amazing touristic resort of El Kantaoui-Sousse in Tunisia.

The organizing committee, in close collaboration with the Scientific Committee and with the sections of the Tunisian Chemial Society and various Specialized Groups, prepared an attractive program addressing all the topics of interest in solid-state chemistry. I also want to express my appreciation to the distinguished speakers and researchers who have graciously agreed to share their insights and expertise with us.

We are convinced that this event encourages all attendees to actively engage in discussions, presentations and lectures. This is an opportunity to foster collaboration, share research findings and explore new frontiers in our respective fields.

Our conference will feature nine notable speakers from various countries, who have agreed to contribute to our program. We aim to provide young researchers with an enjoyable yet educational experience that combines science and pleasure. The SCC 2023 Solid Chemistry Conference will put together almost 250 scientists and the program will be filled with 78 oral and 124 poster presentations on various topics in solid state chemistry.

I extend my best wishes to all attendees for a productive scientific meeting and a pleasant stay in El Kantaoui-Sousse, a beautiful tourist destination all year round.

Prof. Adel MEGRICHE

Faculty of Science of Tunis,
University of Tunis El Manar
Chairman of the SCC 2023

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Imed LAAJIMI	*Tunisian Chemical Society*

	SUNDAY 17 DECEMBER 2023	
14.00 – 17.00	**Welcoming participants, distribution of documents and check in**	
17.00 – 17.30	**Opening Ceremony**	
17.50 – 18.30		**Lecture 1** **Kishor Kumar SADASIVUNI** - *Introduced by* Adel MEGRICHE *Center for Advanced Materials, Qatar University, Doha, Qatar* **Electrochemical CO2 Reduction and Hydrogen Generation for Sustainable Environmental Remediation**
19.30		**Dinner**

	MONDAY 18 DECEMBER 2023 (Morning)	
09.00 – 09.40		**Lecture 2** **Rezan DEMIR-CAKAN** - *Introduced by* Mohamed Lotfi EFRIT *Chemical Engineering, Gebze Technical University, Kocaeli, Türkiye* **Na-Se Batteries : An Advancing Energy Storage System**
09.40 – 10.20		**Lecture 3** **Mohamed BOUOUDINA** - *Introduced by* Mehrez ROMDHANE *Energy, Water, and Environment Research Lab, Prince Sultan University, Riyadh, Saudi Arabia* **Multifunctional Nanomaterials for Sustainability – Physicochemical Properties and Applications in Spintronics, Theranostics, and Environmental Remediation**
10.20 – 10.40		**Gathering for the group photo**
10.40 – 11.15		**Poster Session 1 (P 01 - P 30) Alphabetical Order** **Evaluators:** Rezan DEMIR-CAKAN / Roohollah BAGHERZADEH

		Oral Communications - Session 1		**Oral Communications - Session 1**
		Room A **-** Chair: *Fathi TOUATI* Characterization of solid-state materials properties		***Room B*** **-** Chair: *Zouhair KSIBI* Materials for environmental protection
	Com.	*Communicating*		*Communicating*
11.15 – 11.30	**OC-01A**	AISSA Taissir	**OC-01B**	AGREBI Aymen
11.30 – 11.45	**OC-02A**	AYARI Chaima	**OC-02B**	ANTAR Kais
11.45 – 12.00	**OC-03A**	GHODHBANI Ammar	**OC-03B**	ESSOUSSI Houda
12.00 – 12.15	**OC-04A**	JOMAA Ikram	**OC-04B**	ARAR Wafa
12.15 – 12.30	**OC-05A**	CAMARA Magatte	**OC-05B**	BEN SGHAIER Rafika
13.00		**Lunch**		

		MONDAY 18 DECEMBER 2023 (Afternoon)		
15.00 – 15.40		**Lecture 4** **Deepalekshmi PONNAMMA** - *Introduced by* Latifa BERGAOUI *Research Quality Section, Research Planning and Development Department, Qatar University, Doha, Qatar* **Nanomaterials to Clean Energy : Electrospun Polymer Composites as Nanogenerators**		
		Oral Communications - Session 2		**Oral Communications - Session 2**
		Room A **-** Chair: *Habib BOUGHZALA* Characterization of solid-state materials properties		***Room B*** **-** Chair: Haykel GALAI Materials for environmental protection
	Com.	*Communicating*		*Communicating*
15.45 – 16.00	**OC-06A**	KHACHROUM Hajer	**OC-06B**	CHERBIB Siwar
16.00 – 16.15	**OC-07A**	MAKHLOUF Jawher	**OC-07B**	ELAISSAOUI Ines
16.15 – 16.30	**OC-08A**	MASTOURI Oumaima	**OC-08B**	KTARI Nadia
16.30 – 16.45	**OC-09A**	MRAD Houda	**OC-09B**	OULED MOHAMED Mariem
16.45 – 17.00	**OC-10A**	MZID Massara	**OC-10B**	SAMB Issa
17.00 – 17.45		**Coffee Break & Poster Session 2 (P 31 - P 62) Alphabetical Order** **Evaluators:** Kishor Kumar SADASIVUNI / Mohamed ABDEL SALAM		
		Oral Communications - Session 3		**Oral Communications - Session 3**
		Room A **-** Chair: *Mekki ABDELMOULEH* Advances in solid-state materials synthesis		***Room B*** **-** Chair: *Najoua SRASRA* Materials for renewable energy production & storage
	Com.	*Communicating*	*Com.*	*Communicating*
17.45 – 18.00	**OC-11A**	SOUEMTI Ahmed	**OC-11B**	BAACHAOUI Sabrine
18.00 – 18.15	**OC-12A**	BAHLOUL Assala	**OC-12B**	BELAKEHAL Rania
18.15 – 18.30	**OC-13A**	FANDOULI Amna	**OC-13B**	BOUCHAOUR Mama
18.30 – 18.45	**OC-14A**	GARCI Fatma	**OC-14B**	JAOUADI Mouna
18.45 – 19.00	**OC-15A**	GAROUI Iheb	**OC-15B**	MERAD Laarej
19.00		**Dinner**		

TUESDAY 19 DECEMBER 2023 (Morning)				
09.00 – 09.40		**Lecture 5** **Roohollah BAGHERZADEH** - *Introduced by* Latifa LATROUS *Institute for Advanced Textile Materials and Technologies, Amirkabir University of Technology (Tehran Polytechnic), Tehran, Iran* **Flexible Hybrid Structure Piezoelectric Nanogenerator Based on Organic/Inorganic Nanocomposites Fibrous Materials**		
09.40 – 10.20		**Lecture 6** **Shahzada AHMAD** - *Introduced by* Mohamed DAMMAK *BCMaterials, Basque Center for Materials, applications & Nanostructures, University of Basque Country Science Park, Leioa, Spain* **Light-Matter Interaction in Emerging Photovoltaics**		
10.20 – 11.00		**Poster Session 3 (P 63 - P 94) Alphabetical Order** **Evaluators:** Camara Magatte / Issa Samb		
		Oral Communications - Session 4		**Oral Communications - Session 4**
		Room A **-** Chair: *Mohamed ABDELHEDI* Advances in materials synthesis, functional materials		***Room B*** **-** Chair: *Lilia KTARI* Nano materials
	Com.	*Communicating*		*Communicating*
11.00 – 11.15	**OC-16A**	MAHBOULI RHOUMA Najla	**OC-16B**	ABBASSI Hamed
11.15 – 11.30	**OC-17A**	KHMIRI Mariem	**OC-17B**	AMINI Jinine
11.30 – 11.45	**OC-18A**	MSAOURA Selma	**OC-18B**	AOUINA Aroua
11.45 – 12.00	**OC-19A**	HAJJI Asma	**OC-19B**	KARAFI Athar
12.00 – 12.15	**OC-20A**	JRADI Safi	**OC-20B**	MHADHBI Mohsen
12.15 – 12.30	**OC-21A**	MESSAI Amel	**OC-21B**	RABTI CHAIBI Amal
13.00		**Lunch**		

TUESDAY 19 DECEMBER 2023 (Afternoon)				
		Oral Communications - Session 5		**Oral Communications - Session 5**
		Room A **-** Chair: *Saida SOMRANI* Preparation and synthesis of new inorganic solids		***Room B*** **-** Chair: *Wafa SASSI* Preparation, metal, photonic and optical properties, solid thin film
	Com.	*Communicating*		*Communicating*
15.00 – 15.15	**OC-22A**	DRIDI Rihab	**OC-22B**	SLAMA Marwa
15.15 – 15.30	**OC-23A**	HARZI Feriel	**OC-23B**	DALY Rakia
15.30 – 15.45	**OC-24A**	KHLIFI Ismail	**OC-24B**	ABID Hedia
15.45 – 16.00	**OC-25A**	KOCHBATI Najla	**OC-25B**	FERSI Riadh
16.00 – 16.15	**OC-26A**	GUERMASSI Youssef	**OC-26B**	ABID Kawthar
16.15 – 16.30	**OC-27A**	JANGHER Abdulhakim	**OC-27B**	DAGHAR Chaima
16.30 – 17.15		**Coffee Break & Poster Session 4 (P 95 - P 127) Alphabetical Order** **Evaluators:** Deepalekshmi Ponnamma / Laarej Merad		
		Oral Communications - Session 6		**Oral Communications - Session 6**
		Room A **-** Chair: *Mohamed BELHOUCHET* Preparation, synthesis of new inorganic solids		***Room B*** **-** Chair: *Noureddine RAOUAFI* Sustainable, emerging, biomaterials, solid electrochemistry and corrosion science
	Com.	*Communicating*		*Communicating*
17.15 – 17.30	**OC-28A**	LOUATI Myriam	**OC-28B**	MJAIED Sawsen
17.30 – 17.45	**OC-29A**	MSAADI Radhia	**OC-29B**	MKADMINI Khaoula
17.45 – 18.00	**OC-30A**	MTAR Soulayma	**OC-30B**	YAHIA Achwak
18.00 – 18.15	**OC-31A**	TABABI Intissar	**OC-31B**	ROUIN Ghada
18.15 – 18.30	**OC-32A**	FKIRI Anis	**OC-32B**	CHOUCHENE Mohamed Amine
18.30 – 18.45	**OC-33A**	ACHECH Amel	**OC-33B**	WANNASSI Jassem
19.00		**Dinner**		

WEDNESDAY 20 DECEMBER 2023				
09.00 – 09.40		**Lecture 7** **Mohamed ABDEL SALAM** - *Introduced by* Béchir CHAOUACHI *Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia* **Application of nanotechnology in chemistry, engineering, and biological science**		
		Oral Communications - Session 7		**Oral Communications - Session 7**
		Room A **-** Chair: *Nadia KTARI* Computation, modelling, design		***Room B*** **-** Chair: *Dalila HELLALI* Materials for renewable energy production & storage
	Com.	*Communicating*		*Communicating*
09.45 – 10.00	**OC-34A**	GARA Rayene	**OC-34B**	BELGHAIEB Jalel
10.00 – 10.15	**OC-35A**	JENDOUBI Abir	**OC-35B**	OUESLATI Adel
10.15 – 10.30	**OC-36A**	MAALEJ Ramzi	**OC-36B**	ZAAFOURI Walid
10.30 – 10.45	**OC-37A**	RAHALI Emna	**OC-37B**	RAOUAFI Amal
		Oral Communications - Session 8		
		Room A **-** Chair: *Halim HAMMI* Glasses, ceramics, polymeric materials		
	Com.	*Communicating*		
11.00 – 11.15	**OC-38A**	HAJRI Imen		
11.15 – 11.30	**OC-39A**	MECHICHI Rania		
11.30 – 11.45	**OC-40A**	SEBOUI Zeineb		
11.45 – 12.00	**OC-41A**	GUESMI Sondes		
12.00		**Closing Remarks and Poster Awards**		
13.00		**Lunch, Check Out and Departure**		

Speakers' Abstracts

Kishor Kumar SADASIVUNI

Dr. Kishor Kumar Sadasivuni is an accomplished Research Assistant Professor and the esteemed leader of the SmartNano Solutions group at the Center for Advanced Materials, Qatar University. With a strong foundation in analytical chemistry, he embarked on his academic journey, earning a Master's degree from Andhra University, India. His pursuit of knowledge led him to the University of South Brittany in Lorient, France, where he earned his Ph.D. in Materials Science and Engineering in 2012 under the guidance of Professor Yves Grohens. This marked the beginning of his impressive career in academia and research. Dr. Kishor Kumar Sadasivuni's contributions to the scientific community have been exceptional. His groundbreaking work earned him recognition as one of the world's top 2% scientists, a distinction conferred by Stanford University in 2019, 2020, and 2022. Qatar University has also acknowledged his remarkable achievements with honors. Boasting over 15 years of active research experience, Dr. Kishor has made significant strides in his field. His prolific publication record includes more than 350 research articles in esteemed international peer-reviewed journals, accumulating an impressive total citation count of 13,279 and an h-index of 62. He has also authored 20 book chapters and served as the editor of 11 books, with several of his works featured in Springer's prestigious Top 25 e-book downloads of 2020. Dr. Kishor's innovative mindset is evident through his patent portfolio. He holds three US patents and two Indian patents, with five patent disclosures currently under consideration. As a visionary leader, he spearheads 11 research projects, encompassing grants from the Qatar National Research Fund, including NPRP, UREP, IRCC grants, as well as projects supported by Qatar University, collectively amounting to an impressive 5 million USD. A true collaborator, Dr. Kishor has actively engaged with researchers from diverse disciplines worldwide, boasting over 450 co-authors in fields such as computer science, biomedical sciences, industrial engineering, and electrical engineering. His global collaborations span countries like the USA, France, South Korea, Oman, Spain, Italy, Australia, and Malaysia.

In summary, Dr. Kishor Kumar Sadasivuni is a distinguished figure in the world of academia and materials science, renowned for his prolific research contributions, innovative patents, and extensive collaborative efforts. His dedication to advancing knowledge and fostering international cooperation underscores his commitment to the scientific community.

Electrochemical CO_2 Reduction and Hydrogen Generation for Sustainable Environmental Remediation

Kishor Kumar Sadasivuni[a, b], Muni Raj Maurya[a,] Mizaj Shabil Sha[a]

[a)] *Center for Advanced Materials, Qatar University, P. O Box 2713 Doha, Qatar.*
[b)] *Department of Computer Science and Engineering, Qatar University, PO Box 2713, Doha, Qatar*

Functional nanomaterials play a crucial role in various energy-related applications, including carbon dioxide (CO_2) reduction and hydrogen production. Carbon dioxide is the iconic greenhouse gas and the major factor driving global climate change, incentivizing its capture and conversion to valuable products. Further, atmospheric CO2 levels can be reduced by minimizing the dependence on conventional energy sources. Hydrogen energy technologies parade as promising sustainable solutions to the energy demand at the industrial scale. At present, heterogeneous hydrogenation catalysis and electrocatalysis have the greatest promise for large-scale CO_2 reduction to fuel products and hydrogen production by electrochemical water splitting. Nanocomposite exhibits synergistic effects, leading to improved catalytic activity for carbon dioxide reduction and hydrogen production. Our research focused on nanomaterials like metal oxide, 2D-materials composite and metal-organic frameworks, etc., as catalysts in the electrochemical reduction of CO_2-to-fuel and hydrogen generation. Operating, selectivity and stability conditions were optimized to extract maximum productivity. Further, prototypes were developed and examined for real-time application using renewable energy sources.

Key words: Carbon dioxide reduction, Hydrogen production, Nanomaterial, Electrochemistry

Rezan DEMIR-CAKAN

Rezan Demir-Cakan received her Ph.D. degree at the Max Planck Institute of Colloids and Interfaces (2009). Then in the group of Jean-Marie-Tarascon, she focused on the rechargeable lithium batteries, more specifically on lithium-sulphur batteries between 2009-2012 as a postdoc researcher. Currently she has been working as a Full Professor at the Chemical Engineering Department of Gebze Technical University (Kocaeli/Türkiye). Her current research focuses on the synthesis of nanostructured energy materials and their application in the field of rechargeable batteries. She has received several awards including; French Embassy Fellowship (2023, 2018), Turkish Academy of Science, Distinguished Young Scientist Award (2018), L'Oreal Türkiye Young Women in Science (2016), The Science Academy Young Scientist Award (2015), Young Investigator Award of IMLB (2012) and the Japan Carbon Award (2008). She has been funded by numerous national and international research projects and has co-authored >80 papers in international peer reviewed journals (total citation: >5500, h-index: 30). Since 2014 she has been working as an expert in EU funded projects (H2020, HE) on energy related calls.

Na-Se Batteries : An Advancing Energy Storage System

Zeynep ERDOL[a,b], Ali ATA[a], Rezan DEMIR-CAKAN[c],

[a)] *Material Science and Technology, Turkish-German University, Istanbul, Türkiye*
[b)] *Materials Science and Engineering, Gebze Technical University, Kocaeli, Türkiye*
[c)] *Chemical Engineering, Gebze Technical University, Kocaeli, Türkiye*

With their high volumetric capacity and electronic conductivity, sodium-selenium (Na-Se) batteries have attracted immense attention for advanced battery systems and significant progress has been made in the design of state-of-the-art Na-Se batteries in recent years. However, these battery systems still face some significant obstacles, such as severe volume changes during the discharge-discharge process and uncontrollable sodium selenide (Na_2Se) deposition. To date, significant efforts have been made to overcome severe volume changes. Herein, to address these issues, various electrocatalysts are introduced to effectively catalyze Na_2Se conversion and improve the utilization of active materials. Furthermore, the development of aqueous-based bio-binder will also be discussed during the presentation.

Key words: sodium-selenium batteries, electrocatalyst, Na_2Se deposition, bio-binders

References

[1] Z Erdol, AC Yüzer, N Kılıç, M Ince, A Ata, R Demir-Cakan, 2023, Journal of Power Sources 579, 233297
[2] Z Erdol, A Ata, R Demir-Cakan, 2023, ChemSusChem, e202300998
[3] Z Erdol, A Ata, R Demir-Cakan, 2022, ChemElectroChem 9 (15), e202200465

Mohamed BOUOUDINA

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Professor Mohamed Bououdina is the Leader of the “Energy, Water, and Environment” Lab at Prince Sultan University in the Kingdom of Saudi Arabia. He holds a PhD in Physics from Grenoble Alpes University - France. He has over 20 years of research and teaching work experience and occupied several positions at leading research institutions and academia, including Institute Neel (CNRS) - France, University of Zaragoza - Spain, National Institute of Advanced Industrial Science & Technology - Japan, Queen Mary University of London and the University of Nottingham - United Kingdom, and University of Bahrain - Bahrain. In addition, he was Visiting Professor at Chinese Academy of Science - China and Petronas University - Malaysia. He has broad background and extensive expertise in Physics, Materials Science & Engineering, Nanotechnology, and Energy, specifically in materials design & fabrication, analytical & spectroscopic characterizations, and properties & performance for cutting-edge technologies. He published over 500 papers in ISI journals with a H-index of 61, over 20 book chapters and 2 indexed books. He presented his research findings at international conferences with over 40 as an invited speaker. Besides, he is reviewer and member of the editorial board of international journals, such as International Journal of Hydrogen Energy. His research projects involved partnership with industry, like Sanyo, Toyota and Mazda in Japan, Timet-UK, DSTL and QinetiQ-Ministry of Defense in the UK, Aramco in KSA, and Garmco in Bahrain. During his career, he established a broad and rich research network with eminent scientists in France, UK, North Africa, GCC, India, China, Malaysia, Turkey, Ukraine, Poland, USA, Sweden, Italy, Spain, and Brazil.

Multifunctional Nanomaterials for Sustainability – Physicochemical Properties and Applications in Spintronics, Theranostics, and Environmental Remediation

Mohamed Bououdina

[a)] *Energy, Water, and Environment Research Lab, Prince Sultan University, Riyadh, Saudi Arabia*
[b)] *Department of Mathematics and Science, Faculty of Humanities and Sciences, Prince Sultan University, Riyadh, Saudi Arabia*

Nowadays, nanomaterials (NMs) gather an immense interest due to their remarkable and unique properties, that can be tuned depending on particle's morphology and size, chemical composition (doping), structural defects (vacancies), as well as surface functionalization. NMs offer a broad range of technological applications, such as energy production, conversion and storage, water treatment, biomedical field, electronics, and so on. Nevertheless, the widespread use of NMs requires particular attention, primarily the assessment of their toxicity on health, environment, and aquatic species.

In this presentation, selected NMs will be presented with primarily focus on (i) diluted magnetic semiconductors (DMSs) for spintronics, explicitly ZnO and CdO; (ii) magnetic ferrites MFe_2O_4 for theranostics; (iii) magnetic nanoparticles (α-Fe_2O_3 and spinel ferrites MFe_2O_4) as efficient adsorbent for heavy metals removal and nanostructured doped TiO_2 thin films for the photodegradation of organic pollutants; and (iv) toxicity of commercial oxides nanoparticles particularly used in cosmetics (ZnO, TiO_2, Fe_3O_4) as well as graphene derivatives. Ab-initio calculations based on density functional theory (DFT) were performed to predict/confirm the electronic structure alongside optical, magnetic, mechanical, and photocatalytic properties of the studied MMs. Bried introduction of recent and future research perspectives will be highlighted like hydrogen (production, storage, and application) and CO_2 (capture and conversion).

Key words: Spintronic, Hyperthermia, Adsorption, Photodegradation, Cell Viability, Density Functional Theory.

Deepalekshmi PONNAMMA

Dr. Deepalekshmi Ponnamma is the Section Head of Research Quality at Qatar Univerity. She is a materials scientist and served previously in the Center for Advanced Materials and College of Arts and Sciences, Qatar University, in various roles. She has a research experience of 13 years with a special focus on polymer nanocomposites and various nanomaterials for advanced applications. Dr Ponnamma has over 110 research articles published in international peer-reviewed journals, with a Google Scholar h-index of 49. Her scientific research interest includes nanoarchitectures, porous structures and polymer composites for energy, electronics and environmental-related applications. The outstanding publications of Dr. Ponnamma are recognized in the international community as she was included in the top 2 % of scientists according to the global list compiled by Stanford University for the consecutive years 2020, 2021 and 2022. She has been teaching Master's courses at Qatar University, guiding students in their theses through advanced topics and fostering a deep understanding of the subject matter.

Dr. Ponnamma's research projects have garnered international recognition, earning accolades for their significant contributions to the respective fields.

Nanomaterials to Clean Energy : Electrospun Polymer Composites as Nanogenerators.

Deepalekshmi Ponnamma

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Sustainable energy resources using flexible polymer nanocomposites is a largely explored area of current research. Electrospun polymer composites in particular are attractive prospects for the creation of nanogenerators, which will allow for the effective conversion of mechanical energy into electrical power. Different polymers such as polyvinylidene fluoride and its co-polymers are reinforced with nanomaterials of various architectures for generating self-powering devices due to their specific polar crystalline phases. Piezoelectric and triboelectric power generation strategies offer ultimate solutions for sustainable green energy generation. Triboelectric nanogenerators using polyvinyl alcohol and polylactic acid filled with metal oxide nanoparticles are useful as biodegradable energy devices as well. Thin film and fiber nanogenerators using the polymer nanocomposites for flexible and wearable electronic applications as self-powering devices will be discussed in this presentation.

Key words: Nanogenerator, Fibers, Composites, Society 5.0

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Roohollah BAGHERZADEH

ROOHOLLAH BAGHERZADEH, PhD, PEng

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Director of Institute for Advanced Textile Materials and Technology,
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Roohollah Bagherzadeh is Associate Professor of Fibrous Materials at Amirkabir University of Technology (Tehran Polytechnic). Dr Bagherzadeh received his doctoral degree from Amirkabir University of Technology (AUT, in Tehran, Iran). Upon graduation, he spent more than 3 years as Post-Doc and visiting scholar at AUT, Deakin University (Australia, 2010-2011), and UNSW (Australia, 2011). He has more than 20 years experiences in education, research, and cooperation with diverse external companies and research institutes with more than 80 peer reviewed publications. He works broadly in the area of correlating and understanding the nanoscopic and macroscopic properties of advanced fibrous materials, with emphases on those for energy harvesting, textile based sensors, functional textile, and clothing for a diverse range of applications, including developing novel flexible nanogenerators and energy scavenging for self-powered microelectronics and flexible conductive and transparent materials. Dr Bagherzadeh is currently the Director of Institute for Advanced Textile Materials and Technologies and head of the Advanced Fibrous Materials Research LAB (AFM-LAB) at AUT.

Flexible Hybrid Structure Piezoelectric Nanogenerator Based on Organic/Inorganic Nanocomposites Fibrous Materials

Roohollah Bagherzadeh

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This talk is aimed to deliver key research approaches on the development of novel hybrid piezoelectric structure based on organic and Inorganic fibrous structures, which eliminate the need for post poling treatment in such hybrid structures. Mechanism of electrical performance enhancement of the hybrid structure is also discussed in this paper. To study the effect of hybridization on piezoelectric performance, different organic and inorganic structures were also fabricated as the active component of nanogenerators. The output power of the hybrid structure was found to be enhanced compared to pristine organic or inorganic nanogenerators. Such simple hybrid device, which does not need to complicate post poling treatment, is a more efficient than previous hybrid nanogenerators for practical applications. This strategy can be considered as an efficient improvement approach to enhance the piezoelectric performance of nanogenerators. These fabrication strategies along with nanofabrication of 1 and 2 dimensional structures are expected to enable various applications in the field of self-powered devices and wearable energy scavenging platforms to harvest mechanical energy from the human activities.

Key words: Hybrid Organic/Inorganic structures, Nanogenerators, flexible devices, Nanostructures.

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2. **R. Bagherzadeh***, *et al*., Wearable and flexible electrodes in nanogenerators for energy harvesting, tactile sensors, and electronic textiles: Novel materials, recent advances, and future perspectives, Materials Today Sustainability, **2023**.
3. Marjan Haghayegh, Ran Cao, Fatemeh Zabihi, **R. Bagherzadeh***, *et al.*, Recent advances in stretchable, wearable and bio-compatible triboelectric nanogenerators, Journal of Materials Chemistry C, 10, **2022**.

Shahzada AHMAD

Shahzada Ahmad is Ikerbasque professor, his scientific interests include materials for energy. From 2012 to 2017 he was program director at Abengoa Research, a corporate research center. His scientific publications list reflects his diverse field of interest in the domain of physical chemistry, and materials science, with a research mission to develop advanced materials for energy application. His work has led to the invitation to speak at scientific or policy-based conferences, inventor of patents, Editor and editorial board member of journals, European research council consolidator grant awardee, elected fellow of the Academies, distinguished visiting professor at HUST, BBVA-Leonardo Fellowship, and chair of the energy conferences. He is a strong advocate for renewable energy and regularly writes popular science articles for the public at large at the leading platforms.

Light-Matter Interaction in Emerging Photovoltaics

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Among the emerging photovoltaics, significant consideration has been given in the last decade to the research and development of perovskite solar cells (PSCs), owing to its intriguing electro-optical features; yet, the commercialization of this material has been hindered by its intrinsic degradation. Initially, methylammonium lead triiodide ($MAPbI_3$) based PSCs gave encouraging results followed by compositional engineering of the perovskites to push the photo-current and open-circuit voltage (V_{OC}). The volatility and phase transformation concern in $MAPbI_3$ and phase segregation in mixed perovskites led to the exploration of formamidinium lead triiodide ($FAPbI_3$) for PSCs fabrication. $FAPbI_3$ has a higher tolerance factor and also induced reliability in PSCs. We have developed a powder methodology for $FAPbI_3$ synthesis, that further suppresses the defects present, and alloying with Cs in $FAPbI_3$ demonstrates a significant boost in proton diffusion rates and stability. Furthermore, we adopted an additivization strategy to overcome the stability challenge. It is paramount to uncover the mechanistic inside and gain a real-time understanding of the links between optoelectronic qualities and their underlying mechanisms to optimize the system further. I will showcase the results from our lab on perovskites, kestrites, and organic semiconductors and how these materials interact with light.

Key words: Semiconductors, Thin-film, Solar cells, Perovskite, Organic Electronics

References

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https://scholar.google.com/citations?hl=en&user=9ntymT4AAAAJ&view_op=list_works&sortby=pubdate

Mohamed Abdel Salam was born 1969 in Cairo, Egypt, where he grew up and was raised to love science. He joined one of the top universities in the region; Ain Shams University, Faculty of Science, by 1986 and decided to specialize in Chemistry as it fascinated his mind, heart and eyes. He obtained a Bachelor of Science (B. Sc.) degree in Chemistry by 1990 among the top list of the department. Salam was then chosen to join the National Research Centre in Egypt, where his research work focused on industrial chemistry, and he obtained his first Master of Science degree (M. Sc.) by 1993. He resigned and joined a Petroleum Company at the Egyptian desert where he learned the practical aspects of petroleum extraction and treatment as well as different methods for corrosion, protection, and monitoring. While working at the petroleum company, he was admitted for the Doctor of Philosophy (Ph. D) program at Ain Shams University where he obtained his first Ph. D. By 1998. Afterwards, he immigrated to Canada, and joined Carleton University at the Canadian capital, Ottawa, where he obtained his second M. Sc. by 2003 in the field of electroanalytical speciation, and his second Ph.D. by 2006 in the field of nanomaterials. Dr. Salam joined Health Canada after his graduation, and then he joined the chemistry department at the Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia by 2007. He is at present a professor of physical chemistry in the chemistry department at the Faculty of Science, King Abdulaziz University, and his research interests focuses on the preparation of new nanomaterials and their potential applications for electrochemical application, environmental remediation, desalination, energy, polymer science, as well as their potential biological applications, and potential toxicity. Prof. Salam registered 5 US patents, authored and co-authored 155 research papers at well-known peer reviewed international journals, and he is among the list of the top 2% of the world scientists for many years. Prof. Salam is among the editorial board of Scientific Reports, Chemical Papers, South African Journal of Chemical Engineering, where he really enjoyed his role as an editor (355 Verified Editor Records), and a frequent reviewer for many well-known scientific journals (302 Verified Peer Reviews). His h-index according to Google Scholar is 45, according to Scopus is 41, and according to the web of science is 39. Salam is married and blessed with a 23 year old son (Omar), and three adorable daughters (Sarah, Sana, and Salma), as well as two lovely cats (Kobe and Simba).

Application of nanotechnology in chemistry, engineering, and biological science

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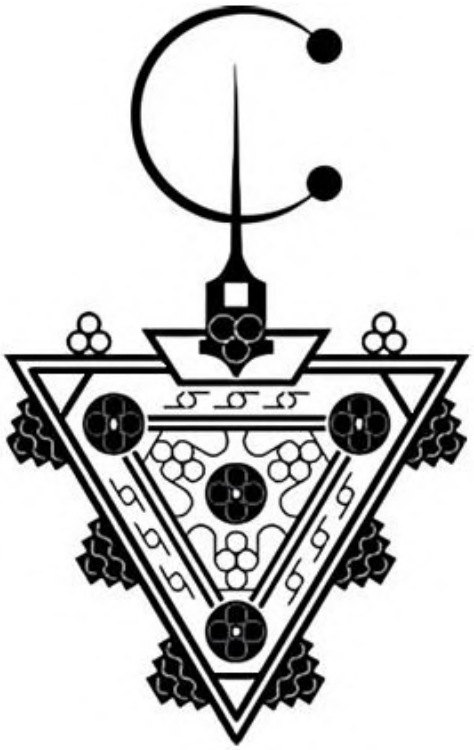
In recent years, nanotechnology has become one of the fastest growing technologies in the world due to significant improvements in the physical, chemical, optical, and mechanical properties of matter reduced to a nanometer size. Currently, nanotechnology is based on the preparation, characterization and applications of different nanoparticles (NPs) such as metals, metal oxides, semiconductors, ceramics, and polymers, due to their outstanding morphological, structural, and physicochemical properties allowed the NPs to be the used in a wide variety of application in chemistry, engineering, and biological science. In this presentation, the applications of nanomaterials, for sustainable environment, sustainable energy, and biology will be presented.

Key words: nanotechnology, nanoparticles, environment, energy, biology



List of Oral Communications

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1	**H. Abbassi**, M. Mezni, R. Abidi, M. Benna-Zayani *FSB - Bizerte* Synthesis and characterization of calix[4]arene diester-grafted functionalized clay nanocomposites	**OC 16B**
2	**H. Abid**, A. Mechria *FSG - Gabès* Synthesis and characterization of α,α'-diimine ligands: A new precursor for novel coordination complexes	**OC 24B**
3	**K. Abid,** A. Samet, S. Pillet, Y. Abid *FSS - Sfax* Tunable Optical Properties In a 2D Organic-Inorganic Hybrid Material	**OV 26B**
4	**A. Achech**, A. Haj Said *FSM - Monastir* $Cu_3(BTC)_2$ hybrid material via conversion of copper (II) hydroxide: Synthesis and caracterization	**OC 33A**
5	**A. Agrebi**, M. Hichri, C. Lafuente *FST - Tunis* Thermophysical properties of deep eutectic solvents based on: Carvone	**OC 1B**
6	**T. Aissa**, D. Aissaoui-Zid, R. Ksiksi, N. Srairi-Abid, M.L Ruck, M.F. Zid *FST - Tunis* Structure, characterization, and in *vitro* antiproliferative effects of a new compound: tetra-[methylimidazolium] dihydrogen decavanadate on IGR39 human melanoma cells	**OC 1A**
7	**J. Amini**, S. Dabbech *LNCM - Tunis* Nanotechnology a promising tool in pharmaceutical industry	**OC 17B**
8	**K. Antar**, M. Jemal *FST - Tunis* Valorization of Tunisian phosphogypsum and raw olive mill wastewaters: a thermogravimetric and kinetic study	**OC 2B**
9	**A. Aouina**, H. Görls, A. Eseola, W. Plass, M.F. Zid, J. Abdelhak *FST - Tunis* Design and Synthesis of Highly Sensitive Fluorophores for Heavy Metal detection	**OC 18B**
10	**W. Arar**, M. Sebai, T. Chabbah, I. Jlalia, N. Jaffrezic-Renault, S. Chatti *INRAP - Sidi Thabet* Effect of the introduction of Isosorbide monomer into linear polymer chains for the removal of aromatic pollutants from water.	**OC 4B**
11	**C. Ayari**, C. Ben Nasr, M.H. Mrad *FSB - Bizerte* A new Zn(II) metal hybrid material of 5-nitrobenzimidazolium organic cation $(C_7H_6N_3O_2)_2[ZnCl_4]$: Elaboration, structure, Hirshfeld Surface, spectroscopic, molecular docking analysis, electric and dielectric properties	**OC 2A**
12	**S. Baachaoui**, W. Mabrouk, O. Ghodbane, N. Raouafi *FST - Tunis* Cost-effective additives for high-performance laser-induced graphene battery-like supercapacitors	**OC 11B**
13	**A. Bahloul**, M. Messaad, M. Abdelhedi *FSS - Sfax* Synthesis, crystal Structure of a novel pyrazolone 3,4-dimethylpyrano[2,3- c]pyrazol-6(2 *H*)-one tested as an acetylcholinesterase inhibitor	**OC 12A**
14	**R. Belakehal**, A. Megriche *INSAT - Tunis* $ZnFe_2O_4$ nano-composite synthesized through ultrasonic-assisted method for enhanced photocatalytic hydrogen evolution	**OC 12B**

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15	**J. Belghaieb**, M.B. Ben Hmida, N. Hajji *ENIG - Gabès* The study of the use of nanofluids to improve the performance of absorbers for refrigerating machines	**OC 34B**
16	**R. Ben Sghaier**, L. Latrous, A. Megriche *CNRSM - Borj Cédria* The potential of animal and vegetable waste for magnetic extraction of Endocrine Disruptors from water	**OC 5B**
17	**M. Bouchaour**, L. Merad, N. Maloufi *University of Tlemcen, Algeria* Improvement of physical properties of ZnO-alloy based for solar cells	**OC13B**
18	**M. Camara**, F. Ngom, C. Daiguebonne, Y. Suffren, K. Bernot, G. Calvez, O. Guillou. *Université Assane Seck de Ziguinchor - Sénégal* Halogen bonds for lanthanide coordination polymers brightness enhancement	**OC 5A**
19	**S. Cherbib**, I. Jlalia, R. Mercier, C. Marestin, S. Chatti, H. Casabianca, N. Jaffrezic-Renault, H. Abderrazak *INRAP - Sidi Thabet* Reversible adsorption efficiency of polyphenols on biobased polymers	**OC 6B**
20	**M.A. Chouchene**, N. Jaouad, N. Amdouni, Y. Chevalier, S. Hbaieb *FST - Tunis* Development of a cyclodextrin-based bio-adsorbent for the removal of pharmaceutical contaminants	**OC 32B**
21	**C. Daghar**, N. Issaoui, H. Marouani *FSB - Bizerte* Synthesis, crystal structure and DFT calculations of novel hybrid organic-inorganic compound, 3-methylbenzylammonium perchlorate	**OC 27B**
22	**R. Daly**, J. J. Sunol, M. Khitouni *FSS - Sfax* Fe-based alloys produced by mechanical milling: structural and thermal characteristics	**OC 23B**
23	**R. Dridi**, B. Esghaier, M.F. Zid, S. Namouchi Cherni *FST - Tunis* Elaboration, structural study and biological activity of a new cadmium complex	**OC 22A**
24	**I. Elaissaoui**, S. Sayeb, H.-Naifer Karima, D. Jellouli Ennigrou *CNRSM - Borj Cédria* Application of acetate cellulose electrospun nanofibers on dye removal	**OC 7B**
25	**H. Essoussi**, H. Barhoumi, S. Karastogianni, S. T. Girousi *FSM - Monastir* An electrochemical sensor based on reduced graphene oxide, gold nanoparticles and molecular imprinted overoxidized polypyrrole for amoxicillin determination	**OC 3B**
26	**A. Fandouli**, A. Houas, A. Rayes *FSG - Gabès* Synthesis, crystal structure, Hirshfeld surface analysis of a new hybrid compound bis(benzylammonium)tetrachlorocadmate(II)	**OC 13A**
27	**R. Fersi**, A.P. Dalia *FST - Tunis* Comprehensive analysis of microstructure and magnetic properties in NdFe/MgO(001) thin films: Influence of thickness and heat treatment	**OC 25B**
28	**A. Fkiri**, M.A. Saidani, A. Chmangui, S. Touil, L. Samia Smiri *FSB - Bizerte* Polyol synthesis of copper doped Gold@ZnO nanorods for the degradation of diuron with solar light in liquid phase	**OC 32A**

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30	**F. Garci**, H. Chebbi, A. Klein, M.F. Zid *FST - Tunis* Structure and comparison of two isomeric; Anti and Syn Cu(II) complexes configuration	**OC 14A**
31	**I. Garoui**, S. Hajlaoui, A. Oueslati *FSS - Sfax* Crystal arrangement and charge transfer mechanisms study of an innovative semiconductor that integrates organic and inorganic elements. $(2A4P)_2SnCl_6$	**OC 15A**
32	**A. Ghodhbani**, Y. Moualhi, R. M'nassri, H. Rahmouni *FSG - Gabès* Validity of some scaling approaches for understanding the electrical response of doped-manganite systems	**OC 3A**
33	**Y. Guermassi**, P. Rudolf, F. Raouafi *FSB - Bizerte* The relevance of catalytic silicate and carbon dust surface reactions in the inner solar nebula	**OC 26A**
34	**S. Guesmi,** V. Bressi, H. Barhoumi, G. Neri *FSM - Monastir* Fe-MOF: A high-performance electrochemical sensor for simultaneous detection of hydroquinone, catechol, and resorcinol	**OC 41A**
35	**A. Hajji,** C. Hernández-Álvarez, A. Souemti, A. Megriche, I. R. Martín *FST - Tunis* Upconversion luminescence for temperature sensing in Er^{3+} doped phosphate materials	**OC 19A**
36	**I. Hajri**, M.R. Ben Romdhane, N. Tessier-Doyen. T. Chartier, E. Srasra *CNRSM - Borj Cédria* Investigations of sintered dry-pressed alumina using synthesized organic copolymer	**OC 38A**
37	**F. Harzi**, N. Fakhar Bourguiba *FST - Tunis* Synthesis, structural and spectroscopic studies, thermal characterization and Hirshfeld surface analysis of cobalt (II) complex $[Co(C_6H_6N_2O)_2(H_2O)_4](NO_3)_2.2H_2O$	**OC 23A**
38	**A. Jangher**, S.K. Shakshooki, F.A. Akari, A.A. Jangher, M.O. Darwish, A.A. Elhammadi, S.A. Elfituri *University of Tripoli, Libya* Physicochemical characterization and electro-conductivity of novel zirconium oxide-crystalline cerium(IV) phosphate/ polybenzimidazole-co-polyaniline, co-polyindole, co-polycarbazole nanocomposites	**OC 27A**
39	**M. Jaouadi**, M. Marzouki, A.H. Hamzaoui, O. Ghodbane *IPEIEM - El manar* Enhanced electrochemical performance of olive stones-derived activated carbon by aluminum coating for supercapacitor applications	**OC 14B**
40	**A. Jendoubi**, M.O. Zouaghi, Y. Arfaoui *FST - Tunis* DFT mechanistic study of the chemical fixation of CO by aziridine derivatives	**CO 35A**
41	**I. Jomaa**, M. Tahenti, N. Issaoui, H. Marouani *FSB - Bizerte* Growth, crystal structure, computational studies, and non-covalent interactions analysis of a novel complex with Cadmium transition metal precursor	**OC 4A**
42	**S. Jradi**, D. Ge, A. Issa, A. Abdelaal, A. Broussier, C. Couteau, S. Blaize, R. Bachelot *University of Technology of Troyes, France* Integration of efficient single photon sources by plasmonic enhanced two-photon polymerization of multifunctional photopolymers	**OC 20A**

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43	**A. Karafi**, L. Baklouti, E. Srasra, B. Mellah *FSB - Bizerte* Coumarins hybridization of Zn (II)-montmorillonite for enhanced fluorescent materials: Spectral and structural characterization	**OC 19B**
44	**H. Khachroum**, M.S.M. Abdelbaky, S.G. Granda, M. Dammak *FSS - Sfax* A new indium hybrid compound based on 2,6-dimethylaniline as ligand: Growth, crystal structure, photoluminescence, and thermal behavior	**OC 6A**
45	**I. Khlifi**, I. Gouti, M. S. M. Abdelbak, S. García-Granda, H. Litaiem *FSS - Sfax* A novel ionic– protonic conductor compound based on tellurium: Synthesis, crystal structure, thermal behavior, Hirshfeld surface analysis, electric and vibrational properties	**OC 24A**
46	**M. Khmiri**, A. Zaouak, C. Belgacem, J. Haikel *CNSTN - Sidi Thabet* Radiation- induced modification of LDPE effects of electron beam accelerator exposure	**OC 17A**
47	**N. Kochbati**, F. Ayari *FSM - Monastir* Sol-gel derived (Zn–)TiO_2 for ultraviolet transmittance: Effect of the surfactant nature on the morphological and structural properties	**OC 25A**
48	**N. Ktari**, M. Manai, M.M. Chehimi *INRAP - Sidi Thabet* Biochar based electrochemical analysis system for drug micropollutant detection	**OC 8B**
49	**M. Louati**, R. Ksiksi, Z. Abdelkafi-Koubaa, N. Srairi-Abid, M.F. Zid *FST - Tunis* Comparison between the antitumor activity of decavanadate compounds	**OC 28A**
50	**R. Maalej,** R. Gargouri, S. Akkoyun, K. Damak *FSS - Sfax* Neutron-induced nuclear cross-section prediction for germanium isotopes via machine learning algorithms	**OC 36A**
51	**N. Mahbouli Rhouma**, A. Dadi, F. Mezzadri, M. Loukil, A. Ghorbal *ISSAT - Gabès* Physico-chemical characterization, Hirshfeld surface analysis and DFT calculation of a hybrid material: 4-(2- ammonioethyl) morpholin-4-ium dichloridodiiodidocadmate/chloridotriiodidocadmate	**OC 16A**
52	**J. Makhlouf**, A. Valkonen, W. Smirani *FSB - Bizerte* Investigation on the molecular, electronic, biological and spectroscopic properties of a novel cobalt complex: An intuition from an experimental and computational perspective	**OC 7A**
53	**O. Mastouri**, O. Kammoun, S. Elleuch, M. Abdelhedi, M. Boujelbene *FSS - Sfax* Hybrid material L-phenylalaninium selenate monohydrate as prospective light-harvesting materials: Synthesis, thermal behavior, vibrational and optical properties.	**OC 8A**
54	**R. Mechichi**, S. Chatti, I. Jlalia, H. Casabianca, E. Vulliet, R. Mercier, S. Weidner, N. Jaffrezic-Renault, H. Abderrazak *INRAP - Sidi Thabet* Poly(ether-sulfone) modified silica gel for the adsorption of water pollutants	**OC 39A**
55	**L. Merad**, A. Slami, M. Bouchaour *University of Tlemcen, Algeria* Investigation of TiO_2 ETM for perovskite based solar cells with different HTMs	**OC 15B**
56	**A. Messai** *Abbes Laghrour University, Khenchela, Algeria* Elaboration of new objects belonging to coordination chemistry and molecular magnetism	**OC 21A**

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59	**K. Mkadmini**, S. Ghwaidia, H. Hammi, A.H. Hamzaoui, T Saied *CNRSM - Borj Cédria* Optimization of an eco-friendly cement mortar by response surface methodology	**OC 29B**
60	**H. Mrad**, S. Akriche *FSB - Bizerte* Enhancement of structural, Spectroscopic and Antimicrobial performance of a novel decavanadate complex $Mg_2(NH_4)_2V_{10}O_{28}.12H_2O$	**OC 9A**
61	**R. Msaadi**, W. Sassi, A.K. Bhakta, S. Ammar, M.M. Chehimi *FSG - Gabès* Preparation and analysis of biochar-ZnO catalyst for electrochemical degradation of Congo Red in wastewater	**OC 29A**
62	**S. Msaoura**, A. Houas, A. Rayes *FSG - Gabès* A new 0-D hybrid bismuth halide compound $(C_{13}H_{28}N_2)_4$ $[BiCl_6]_2$ .2Cl. $5H_2O$: Synthesis, crystal structure and physical properties	**OC 18A**
63	**S. Mtar,** N. Chniba Boudjada, M. Boujelbene *FSS - Sfax* Theoretical and experimental characterizations of a hybrid compound based on peprchlorate salts	**OC 30A**
64	**M. Mzid**, N. Abid, H. El Feki *FSS - Sfax* Antioxidant and antimicrobial activities of ethanol extract from *Spirulina platensis*	**OC 10A**
65	**A. Oueslati** *ISET - Zaghouan* Thermal energy storage processes : Recent applications and innovations	**OC 35B**
66	**M. Ouled Mohamed**, L. Khalfa, M. Bagane *ENIG - Gabès* Removal of antibiotics by adsorption into clay	**OC 9B**
67	**A. Rabti Chaibi**, S. Baachaoui, O. Ghodbane, N. Raouafi *INRAP - Sidi Thabet* Polydopamine modified laser-induced graphene electrodes for capacitive sensing of nitrites ions	**OC 21B**
68	**E. Rahali**, Y. Arfaoui *FST - Tunis* CO_2 adsorption on modified graphene, DFT investigation	**OC 37A**
69	**A. Raouafi,** S. Baachaoui, O. Ghodbane, N. Raouafi *FST - Tunis* Laser-induced graphene interdigitated electrodes modified with redox-active polymers for energy storage	**OC 37B**
70	**G. Rouin**, Y. Ben Amor, M. Abdelmouleh, M. Masmoudi *ENIS - Sfax* Valorization of spent coffee grounds extract as a corrosion inhibitor of copper in NaCl solution	**OC 31B**
71	**I. Samb**, J. Bell, P.Y. Toullec, V. Michelet, I. Leray *Université Alioune Diop, Bambey, Sénégal* Fluorescent sensors for detecting environmentally toxic metal ions	**OC 10B**

Nr.	Authors, Institution and Title of Abstract	Ref
72	**Z. Seboui**, S. Hraiech, H. Hamzeoui *CNRSM - Borj Cédria* Investigation of physical properties of Al doped lead phosphate glasses	**OC 40A**
73	**M. Slama**, K. Issa, K. Ons, M. Ben El Hadj Rhouma *IPEIM - Monastir* Geometrical and relative stabilities of iron oxide clusters Fe_nO_m	**OC 22B**
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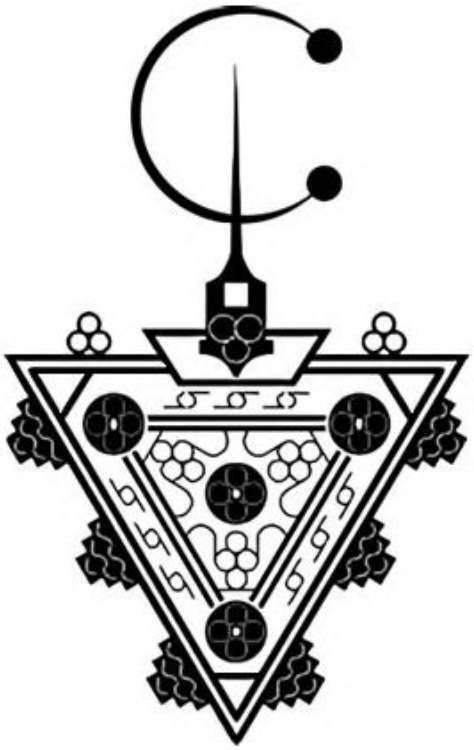

Abstracts of Oral Communications

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Structure, characterization, and in *vitro* antiproliferative effects of a new compound: tetra-[methylimidazolium] dihydrogen decavanadate on IGR39 human melanoma cells

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Melanoma, a malignancy derived from melanocytes, is susceptible to rapid metastasis to other organs if not promptly addressed. It frequently demonstrates inherent resistance to conventional therapeutic approaches [1]. In this regard, new potential drugs are being developed as possible treatments for melanoma. The tetra-[methylimidazolium] dihydrogen decavanadate(V) salt $(C_4H_7N_2)_4[H_2V_{10}O_{28}]$ is characterized by single-crystal X-ray diffraction, by FT-IR, UV-Vis and ^{51}V NMR spectroscopy, as well as by thermal analysis (TGA and DSC). The compound crystallizes in the monoclinic centrosymmetric space group $P2_1/c$. Its formula unit consists of one dihydrogen decavanadate anion $[H_2V_{10}O_{28}]^{4-}$ and four organic 4-methylimidazolium cations $(C_4H_7N_2)^+$. Important intermolecular interactions are N-H···O and O-H···O hydrogen bonds and π-π stacking interactions between the organic cations, revealed by analysis of the Hirshfeld surface and its 2D fingerprint plots. Interestingly, this compound inhibits the viability of IGR39 cells with IC_{50} values of 4 µM and 14 µM after 24 h and 72 h of treatment. Therefore, we could consider it as a new future potential metallodrug against melanoma.

Keywords: Decavanadate, Metallodrugs, Melanoma, IGR39, Anticancer activity

***Funding:** Ministry of Higher Education and Scientific Research of Tunisia (PRF code of this project: **PRF2019-D3P2).**

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A New Zn(II) Metal Hybrid Material of 5-Nitrobenzimidazolium Organic Cation $(C_7H_6N_3O_2)_2[ZnCl_4]$: Elaboration, Structure, Hirshfeld Surface, Spectroscopic, Molecular Docking Analysis, Electric and Dielectric Properties

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The slow solvent evaporation approach was used to create a single crystal of $(C_7H_6N_3O_2)_2[ZnCl_4]$ at room temperature. Our compound has been investigated by single-crystal XRD which declares that the complex crystallizes in the monoclinic crystallographic system with the $P2_1/c$ as a space group. The molecular arrangement of the compound can be described by slightly distorted tetrahedral $ZnCl_4^{2-}$ anionic entities and 5-nitrobenzimidazolium as cations, linked together by different non-covalent interaction types (H-bonds, Cl…Cl, π…π and C–H…π). Hirshfeld's surface study allows us to identify that the dominant contacts in the crystal building are H…Cl/Cl…H contacts (37.3%). FT-IR method was used to identify the different groups in $(C_7H_6N_3O_2)_2[ZnCl_4]$. Furthermore, impedance spectroscopy analysis in $393 \leq T \leq 438$ K shows that the temperature dependence of DC conductivity follows Arrhenius' law. The frequency–temperature dependence of AC conductivity for the studied sample shows one region (E_a = 2.75 eV). In order to determine modes of interactions of compound with double stranded DNA, molecular docking simulations were performed at molecular level.

Key words: zinc (II) complex, hydrogen bonds, AC conductivity, FT-IR, molecular docking study.

Validity of some scaling approaches for understanding the electrical response of doped-manganite systems

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Recently, the discovery of innovative multifunctional perovskites is an imperative topic in the research and development fields. Accordingly, perovskite oxide systems exhibit important electrical and dielectric characteristics that are related to the microstructure, the particle size, and the density of states around the Fermi level [1,2]. In the present work, we investigate the electrical response of a doped manganite ceramic $La_{0.8}Ca_{0.2}Mn_{0.5}Ni_{0.5}O_3$ using the impedance results and some scaling models. Based on the Nyquist plot results, we found that the electrical response of the studied compound is attributed to the main contribution of conductive grains and insulating grain boundary regions. The impedance results confirm that the prepared sample reveals a semiconductor behavior over a large temperature range. In addition, it indicates the presence of relaxation phenomena. The superposition of the conductance spectra confirms the validity of the time-temperature principle (TTSP). At high frequencies, the deviation from the Summerfield scaling superposition indicates that the charge carrier mobility is temperature-dependent. Using the corrected Summerfield scaling model, the deduced $\alpha = 1.2$ parameter indicates the presence of Coulomb interaction between charge carriers.

Key words: Complex impedance analysis, TTSP, Summerfield scaling model

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Growth, crystal structure, computational studies, and non-covalent interactions analysis of a novel complex with Cadmium transition metal precursor

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A novel hybrid material $(C_3H_5N_2)_6[CdCl_4][CdCl_6]$ was successfully synthesized using a slow evaporation process. The structure was confirmed through single-crystal X-ray crystallography, FT-IR, and thermal analysis. The material was found to crystallize in the tetragonal system (space group $I4_1/a$) and the following parameters a=b= 12.0872 (8) Å; c = 24.6985 (16) Å, the crystal packing shows parallel layers of cations and stacks of discrete anions positioned at y = 1/4 and 3/4. The junction between the monoprotonated imidazolium cations and the anions, along with the crystal structure stability, relies on N-H…Cl, and C-H…Cl hydrogen bonds. Computational investigations, conducted using the B3LYP method with 6-311++G(d,p) and LANL2DZ mixed basis set, demonstrated close alignment between the computed and the experimental data, providing insights into the material's geometrical and vibrational properties. The non-covalent interactions were studied through AIM and RDG analysis and quantitatively using the Hirshfeld surfaces associated with 2D fingerprint plots. Furthermore, thermal stability was assessed through TG–DSC analysis.

Key words: Cd(II) complex, DFT calculation, IR spectroscopy, Hirshfeld surface, AIM-RDG.

Halogen bonds for lanthanide coordination polymers brightness enhancement

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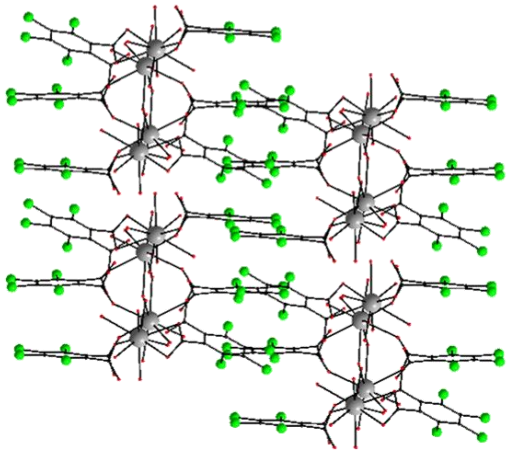
Benzene di-carboxylate ligands have proved their efficiency for the design of large series of isostructural luminescent lanthanide-based coordination polymers.[1] Indeed phenyl rings act both as antenna and as structuring agent via π-stacking interactions. Because lanthanide ions valence orbitals are shielded by filled 5s and 5p orbitals, lanthanide ions have almost no structuring effect and the structuring character of the ligand most often insures the crystal packing. However, beside these beneficial effects, π-stacking is also detrimental because it favors intermetallic energy transfers that are responsible for luminescence intensity decreasing.[2]

Our recent crystallo-chemical studies seem to indicate that the use of halogenated benzene poly-carboxylate ligands could allow to disconnect both effects. Indeed, they strongly suggest that halogen interactions surpass π-π interactions and therefore can lead to crystal packings free from π-stacking. This opens the way to the design of systems in which the beneficial antenna effect of the phenyl ring is preserve while the detrimental non-radiative de-excitation pathways through π-π interactions is absent. Additionally, halogenation of the phenyl rings reduces the number of C-H high energy vibrators in the vicinity of the lanthanide ion that are known for being responsible for non-radiative de-excitation.



Projection view of a lanthanide coordination polymer based on 2,3,4,5-chloro-benzene-1,6-di-carboxylate ligand.

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A new indium hybrid compound based on 2,6-dimethylaniline as ligand: Growth, crystal structure, Photoluminescence, and thermal behavior

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Significant emphasis has been placed on organic-inorganic hybrid materials because of their captivating structures and configurations. These compounds signify a progressive domain within the realm of material science. Significant emphasis has been placed on organic-inorganic hybrid materials because of their captivating structures and configurations.

In this work, a novel hybrid material, formed by combining 2,6-dimethylanilinium cations with (InCl3), has been successfully created and its structure determined using X-ray diffraction. The compound in question is characterized via PXRD and SEM analyses, photoluminescence spectroscopy (PL), and thermal analysis by (DSC) and (DTA/TGA).

The title compound belongs to the triclinic system (*P-1*) space group. The crystal structure contains is built up by sheets of organic cations and octahedral anions alternating by two lattice water molecules. PXRD analysis has been employed to authenticate the crystalline nature of the sample in the solid state. The crystalline nature and the morphology of the product was confirmed by Scanning Electron Microscopy (SEM) and PXRD analyses. The PL spectrum reveals a violet luminescence peak at 289 nm and an intensely blue luminescence one at around 448 nm. Besides, the TGA/DTA analysis shows a thermal stability up to 320 K then it decays in three successive steps, losing a 77,960 % of the total mass. However, the DSC thermogram confirms the results obtained by TGA/DTA analysis.

Key words: SXRD, crystal structure, SEM, PXRD, PL, TGA/DTA, DSC.

Investigation on the molecular, Electronic, Biological and Spectroscopic properties of a novel cobalt complex: An intuition from an experimental and computational perspective

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The preparation, spectroscopic, biological and electrical characterization, in addition of the X-ray crystal structure investigation of a novel tree-dimensional compound $(C_6H_{16}N_2)[Co(NCS)_4]$ is reported. The synthetized compound crystallizes in the $P2_12_12_1$ space group. The structure is made up of layers of cobalt (II) bridged by thiocyanate-N ligand **[1].** The vibrational modes of the functional groups were investigated using FT-IR measurements. Hirshfeld surface analysis was performed to investigate the short contacts and hydrogen bonds in the compound. In addition of the study of the photoluminescent behavior which reveals a high optical property **[2].** Explorations of impedance spectroscopy on $(C_6H_{16}N_2)$ $[Co(NCS)_4]$ reveal fascinating electrical behavior **[3].** Finally, the compound's antioxidant activity and the molecular docking were occurred which suggest that the Cobalt complex acts as a COX-2 inhibitor Agent **[4].**

Key words: Materials chemistry, X-ray structure determination, DFT, impedance spectroscopy, Antioxidant activity, Molecular docking.

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Hybrid Material L-phenylalaninium Selenate Monohydrate as Prospective Light-Harvesting Materials: Synthesis, Thermal behavior, Vibrational and Optical properties

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The present work focuses on the study of a new organo-selenate hybrid material namely $[C_9H_{12}NO_2]_2SeO_4.H_2O$, which was abbreviated $(LPA)_2.SeO_4.H_2O$, was successfully obtained by an acid-base reaction at room temperature by slow evaporation. The crystal structure that was studied by the X-ray single-crystal diffraction process was crystallized in the monoclinic system whose space group is non-centrosymmetric $P2_1$ with the following lattice parameters: a = 12.817(3) Å; b = 6.2716(15) Å; c = 13.629(3) Å, β=103.847(7) °, Z= 2 and V= 1063.7 (4) $Å^3$. The atomic arrangement in the crystal structure was described as an alternation of organic and inorganic entities along the a-axis. The IR and Raman spectra were recorded in the 500-4000 cm^{-1} and 0-4000 cm^{-1} frequency region, respectively, confirmed the existence of vibrational modes that correlate with organic and inorganic groups. Crystal arrangement is determined by hydrogen bonds of the type N-H…O, O-H…O and OW-H…O. The intermolecular interactions in the crystal structure were performed and analyzed using Hirshfeld surface analysis. DSC-TGA analysis have shown that compound dehydration at around 90°C, produced an anhydrous compound that is thermically stable between 90°C and 122°C. The experimental UV-Visible absorption of the compound's optical properties demonstrated its semiconducting properties, revealed a direct optical band gap at 5.53 eV. Finally, photoluminescence measurements indicate that the synthesized material exhibits solid-state luminescence properties.

Enhancement of structural, Spectroscopic and Antimicrobial performance of a novel decavanadate complex $Mg_2(NH_4)_2V_{10}O_{28}.12H_2O$

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An assemblage between NH_4VO_3 and $Mg(CHCOO)_2.H_2O$ in aqueous solution gives rise to a novel decavanadate complex. Single crystal X-ray diffraction shows that the complex $Mg_2(NH_4)_2V_{10}O_{28}.12H_2O$ crystallizes in the triclinic system with the P1 space group and the following lattice parameters : a = 8.5080 (8) Å, b = 10.4269 (9) Å, c = 11.2982 (10) Å, α = 68.526 (3)° β = 87.269 (3)°, γ = 67.143 (3)° V = 854.23 (13) $Å^3$. In addition, Hirshfeld surface analysis was performed to investigate the short contacts and hydrogen bonds in the compound.

Furthermore, the resulting compound was characterized by FT-IR measurements to determine its vibrational modes. The electronic transitions and the gap energy study was occurred using UV-visible spectroscopy [1]. Finally, the $Mg_2(NH_4)_2V_{10}O_{28}.12H_2O$ material was evaluated for its antimicrobial behavior in both bacterial and fungal pathogens of clinical potential [2].

Key words: Crystal structure, X-Ray Diffraction, Spectroscopy, UV-Visible, FT-IR, Hirshfeld surface, Antimicrobial Activity.

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Antioxidant and antimicrobial activities of ethanol extract from *Spirulina platensis*

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Spirulina platensis (SP) is a well known medicinal plant used in Tunisia against several diseases [1]. This study was devoted to the determination of polyphenols, flavonoids, and flavonols contents of SP after their extraction using aqueous ethanol (75%), as well as the determination of the content of macro and micro elements, the antioxidant and the antimicrobial activities of the extract. The results obtained indicate that the aqueous ethanol (75%) extracts presented highest contents of polyphenols. The antioxidant activity was evaluated using DPPH radical scavenging activity and chelating of ferrous ions tests. Fourier Transform Infrared Spectrometry (FTIR) and Thermogravimetric analysis (TG) of SP was also evaluated.

The proximate analysis showed that SP contained appreciable percentages of bio elements. The results showed that ethanol extract has diverse antioxidant capacities. The extract was screened for antibacterial and antifungal activities. Ethanol extract had good and antibacterial effects against standard strains of *Bacillus cereus* ATCC 14579, *Pseudom*onas *aeruginosa* ATCC 9027, *Staphylococcus aureus* ATCC 29213, and *Escherichia coli* ATCC 8739. Ethanol extract was the most effective with minimum inhibitory concentration <150 mg/ml against *Staphylococcus aureus, Micrococcus luteus, Pseudomonas aeruginosa, Klebsiella pneumoniae, Bacillus cereus* and *Enterococcus faecalis*. The extract showed antifungal activity against *Candida albicans* ATCC 10231 and *Aspergillus brasiliensis* ATCC 16404.

FT-IR analysis represents functional groups in SP and The TG curve made it possible to describe the thermal analysis of SP.

The results of the present work indicate that SP extract could be used as natural antioxidant and antimicrobial agents in the food preservation and human health.

Key words: *Spirulina platensis*, antimicrobial activity, antioxidant activity, FTIR

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Luminescence and electrical properties of rare earth doped polyphosphate materials

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In the present work, we have successfully synthesized polyphosphate materials, pure and doped with rare earths elements, with chemical formula $KMg_4(PO_4)_3$ by high-temperature solid solution method. The resulting pure phases crystallized in the simple orthorhombic system Pnnm. X-ray diffraction and IR spectroscopy characterizations confirm the high purity of the phase and incorporation of the lanthanide element in the crystal structure, on the one hand, and high thermal stability, on the other hand. Optical property analyses show that such materials can be used as in light-emitting diodes LEDs application domain. The electrical properties indicate ionic conductivity at intermediate temperatures, making them suitable as electropositive electrode materials for electrochemical batteries.

Keywords: Alluaudite materials, Orthophosphates, Optical properties, Semi-ionic conductor, Impedance Spectroscopy.

Synthesis, crystal Structure of a novel pyrazolone 3,4-dimethylpyrano[2,3- *c*]pyrazol-6(2 *H*)-one tested as an acetylcholinesterase inhibitor

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Pyrazolone derivatives have various applications in different fields, making them increasingly popular. The objective of this study is to develop a new anti-Alzheimer's drug and compare it with the reference compound, rivastigmine, against human acetylcholinesterase (AChE). The compound was obtained with good yield and was characterized by spectral technique such as ^{1}H NMR, ^{13}C NMR, FT-IR and X-ray crystallography.

Single-crystal X-ray study showed that the structure of pyrazolone derivative $C_8H_8N_2O$ is crystallized in the monoclinic space group P 2_1/n, with the following parameters a = 13.536 (7) Å, b = 15.852 (9) Å, c = 11.354 (5) Å, β= 95.314 (2) °, Z = 8 and V = 1470.59 (14) Å^3.

This compound was evaluated for its inhibitory effect against AChE implicated in the development of Alzheimer's disease using the in silico study, it was occupying the site located in the deep cavity of AChE and rivastigmine was occupied the central active site cavity of AChE. The detailed interactions between the rivastigmine and the synthesized compound and human acetylcholinesterase were deter- mined and showed that the AChE- compound complex was established several interactions with catalytic residues (His 447 and Ser 203) and the critical residue for the inhibition of the human enzyme (Tyr 337).

The *in vitro* Acetyl- cholinesterase (AChE) inhibition studies showed that the synthesized compound has a good inhibitory activity against AChE and this activity is similar to that of rivastagmine with an IC 50 value of 0.38 ±0.019 mg/mL ($p < 0.05$) and 0.36 ±0.018 mg/mL ($p < 0.05$), respectively.

According to the results in the in silico and in vitro studies, this compound has potential for in vivo anti-Alzheimer evaluations.

Keywords: Pyrazolone, Acetylcholinesterase (AChE) inhibitors, Molecular docking.

Synthesis, crystal structure, Hirshfeld surface analysis of a new hybrid compound Bis(benzylammonium)tetrachlorocadmate(II)

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The synthesis of organic-inorganic hybrid materials represent one of the most active areas of materials science and chemical research [1] as there is a growing interest in developing materials with specific characteristics not found in a single constituent which can be a promising solution in a number of applications [2]. A new non-centrosymmetric hybrid material, (C6H5CH2NH3)2CdCl4, was synthesized, by slow evaporation method at room temperature (RT). Single-crystal X-ray diffraction (SC-XRD) analysis showed that the material crystallized at RT in orthorhombic system with space group Cmca and the following unit cell parameters a = 7.5047(5) Å, b = 33.070(2) Å, c = 7.5791(5) Å,V = 1881.0(2) Å3 and Z = 4. The asymmetric unit of the crystal consists of an isolated anion (CdCl4) 2- and a protonated benzylamine disordered with two possible orientations around a crystallographic special position. Such crystallographic disorder phenomenon prompted us to determine the structure of this compound at low temperatures. The crystal structure does not retain the same space group symmetry over a wide temperature range, as shown by single crystal analyses performed at 100, 200 and 298 K. In fact, at 100 K this material crystallizes in the monoclinic system with space group Cc and the cation is found in two different positions in the asymmetric unit. At 200 K, this material crystallizes in orthorhombic system with space group Aba2. Each allotropic variety consists of corner-sharing distorted CdCl6 octahedra forming two-dimensional layers stacked in a staggered fashion. Benzylammonium cations C7H7NH+ are located in the interlayer spacing and link adjacent inorganic layers via charge-assisted weak hydrogen bonds between the ammonium -NH3 + moieties and Chloride ions. Hirshfeld surfaces and their associated 2D fingerprint plots were used to explore and quantify the intermolecular interactions in the crystal lattice of the title compound. The new title compound is also characterized by FT-IR spectroscopy and thermal analysis.

Key words: Organic-inorganic hybrid material; Crystal structure; thermal analysis; Hirshfeld surface analysis.

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Structure and comparison of two isomeric; *Anti* and *Syn* Cu(II) complexes configuration

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Two isomeric 2-bromomethylpyridine Cu(II) complexes $[Cu(C_6H_9NBr)_2(NO_3)_2]$ with 2-bromo-5-methylpyridine (**L^1**) and 2-bromo-4-methylpyridine (**L^2**) were synthesized as air-stable blue materials in good yields. In both cases, X-ray single crystal diffraction showed a primary *trans*-N_2(Py)O_2(NO_3) coordination of the Cu(II) centers. The crystal structures were different with $[Cu(L^1)_2(NO_3)_2]$ (**CuL^1**) crystallized in the monoclinic space group $P2_1/c$, while the 4-methyl derivative **CuL^2** was solved and refined in the triclinic space group $P\bar{1}$. Also the orientation of the Br substituent in the molecular structure (*anti* (**CuL^1**) and *syn* (**CuL^2**) configurations).

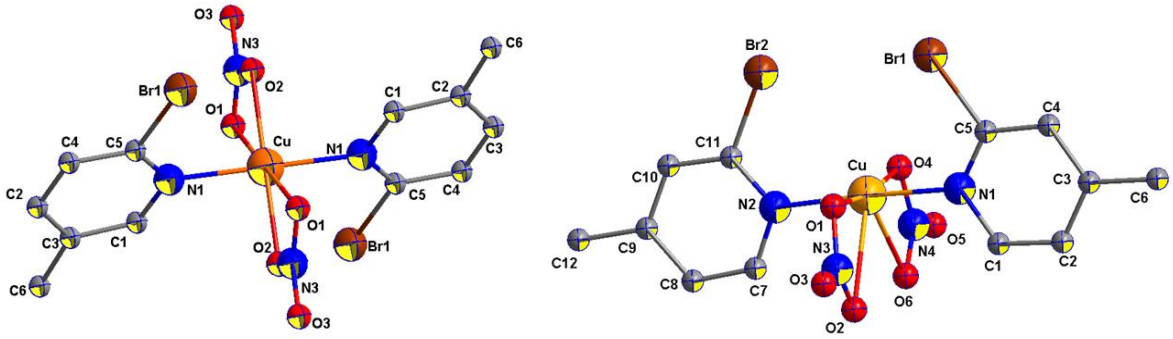

Figure: *The asymmetric unit of the two forms of $[Cu(L)_2(NO_3)_2]$ with numbering. Left:* ***CuL^1****, right:* ***CuL^2***

Key words: Copper, Syn, Anti, stereoisomers.

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Crystal arrangement and charge transfer mechanisms study of an innovative semiconductor that integrates organic and inorganic elements (2A4P) $_2SnCl_6$

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A novel organic-inorganic hybrid compound, named bis-2-amino-4-picolinium hexa-chlorostannate (2A4P) $_2SnCl_6$, has been successfully synthesized and characterized using single-crystal X-ray diffraction, differential scanning calorimetry (DSC) and complex impedance spectroscopy. At room temperature, the compound crystallizes in the centrosymmetric $P2_1/c$ space group. The analysis of complex impedance spectra shows that the material's electrical properties are strongly influenced by frequency and temperature, indicating a relaxation phenomenon and semiconductor-like behavior. When a high relative density pellet is used for electrical measurements, a single semicircle is detected in the complex impedance spectra, which can be adequately fitted with a combination of resistance (R), capacitance (C), and constant phase element (CPE) elements representing the bulk response. The findings of a charge transportation study in (2A4P) $_2SnCl_6$ point to the presence of the correlated barrier hopping CBH model. Overall, the research sheds light on the synthesis, crystal arrangement and charge transfer mechanisms in this novel semiconductor, emphasizing its electronic potential.

Keywords: Inorganic materials, Crystal growth, X-ray diffraction, CBH model.

Thermophysical properties of deep eutectic solvents based on: Carvone

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Due to their importance, organic solvents are widely used compounds in many professional applications. On the other hand, no organic solvent is harmless, they all have health effects. They enter the body mainly through the respiratory route and also through the skin and can thus cause damage to the nervous system (dizziness, drunkenness, paralysis, etc.), skin conditions (irritation, burning, dermatosis), blood (anemia), liver (hepatitis), kidneys. In addition to health risks, there is the risk of fire and explosion.

For many years, these shortcomings accompanying conventional organic solvents have caused their exclusion from the framework of green chemistry and have prompted scientific research and particular attention is paid to the development of new generations of solvents that are more respectful of the environment. As such, Deep Eutectic Solvents (DESs) are attracting growing interest.

Deep eutectic solvents (DESs) are mixtures of Hydrogen Bond Donnor HBD and Hydrogen Bond Acceptor HBA, composed of two or more solid or liquid components that form a eutectic mixture with a lower melting point than the individual components. Unlike conventional solvents (ethanol, methanol ...), deep eutectic solvents are non-volatile, which means that they have a very low vapor pressure and are therefore hardly flammable. The toxicity of deep eutectic solvents is low, their biodegradability is high, and the necessary precursors are inexpensive, easily and abundantly available as well as renewable. Given their economic, medical and environmental interest, the thermophysical study seems essential to reveal the thermal behavior and the physical properties of these solvents.

Through this work, several thermophysical properties of binary liquid mixtures based on Carvone, have been measured, on different molar ratio.

A study of the refractive index, density and speed of sound, Viscosity and Surface tension were made on each synthesized composition whose molar fractions are (1:2, 1:1, 2:1) of the following three systems (carvone-thymol, carvone-decanoic acid, carvone-octanoic acid) as a function of temperature and at atmospheric pressure (P = 0.1 MPa).

Valorization of Tunisian phosphogypsum and raw olive mill wastewaters: A thermogravimetric and kinetic study

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Large amounts of phosphogypsum (PG) and olive mill wastewaters (OMW) are rejected regularly in the environment. This work aimed at the valorization of both PG and OMW from Tunisia in order to recover calcium sulfide. It consists in studying the reduction of the former using the latter as a source of carbon in nitrogen atmosphere. Experiments were carried out by thermogravimetry in non-isothermal mode and the solids were identified by X-Ray diffraction. Raw samples (OMWR) of OMW were used and the PG over OMWR mass ratio were varied to find the stoichiometric proportion of the reaction between $CaSO_4$ and carbon. It was found that in pure N_2 atmosphere the use of OMWR as carbon source, allows to significantly reduce both the onset reduction temperature and the reduction temperature interval: the PG reduction takes place in the temperature range of 600°C-750°C [1] (instead of 750°C-1080°C with pure Carbon) [2] leading to calcium sulfide (CaS) formation. Utilizing Kissinger-Akahira-Sunose, Flynn-Wall-Ozawa, Kissinger, Šatava-Šesták and master plots methods allow to the determination of activation energies, pre-exponential factors and the mechanism models of the reduction reaction. The results suggest that calcium sulfate reduction can be described by a single-step process. The best model for the PG + OMWR at 0.23 mass ratio mixture was Avrami-Erofeev A2. The kinetic models corresponding to this mixture is:

$$\frac{d\alpha}{dt} = 1.32 \times 10^{12}\, exp\left(-\frac{214.92 \times 10^3}{RT}\right) \times 2(1-\alpha)(-ln(1-\alpha))^{1/2}.$$

Keywords: Calcium sulfide, phosphogypsum, olive mill wastewaters, TG, FWO and KAS isoconversional methods, Šatava-Šesták, mater plots, activation energy.

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An Electrochemical Sensor Based on Reduced Graphene Oxide, Gold Nanoparticles and Molecular Imprinted Overoxidized Polypyrrole for Amoxicillin Determination

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An electrochemical sensor for amoxicillin (AMX) detection based on reduced graphene oxide (RGO), molecular imprinted overoxidized polypyrrole (MIOPPy) modified with gold nanoparticles (AuNPs) is described in this work. The electrochemical behavior of the imprinted and non-imprinted polymer (NIP) was carried out by cyclic voltammetry (CV). The morphology of the prepared MIP sensor were characterized by scanning electron microscopy (SEM) and its experimental parameters such as monomer and template concentration, pH buffer solution, incubation time of AMX and AuNPs, scan rate as well as electropolymerization scan cycles were optimized to improve the performance of the sensor. The peak current obtained at the MIP electrode was proportional to the AMX concentration in the range from 10^{-8} to 10^{-3} mol L^{-1} with a detection limit and sensitivity of 1.22 10^{-6} mol L^{-1} and 2.52× 10^{-6} µAmol^{-1} L, respectively. It was also found that this sensor exhibited an excellent selectivity against molecules with similar chemical structures. Besides, the analytical application of the AMX sensor confirms the feasibility of AMX detection in milk.

Keywords: Amoxicillin, molecular imprinted overoxidized polypyrrole, gold nanoparticle, reducer graphene oxide, cyclic voltammetry.

Effect of the introduction of Isosorbide monomer into linear polymer chains for the removal of aromatic pollutants from water.

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The pollution of water resources with organic compounds such like phenols, dyes, pesticides, and pharmaceuticals, became a serious challenge to overcome due to the direct toxicological effect on aquatic life and human health [1, 2]. For the removal of these contaminants from wastewater, different effective techniques have been developed, including chemical coagulation [3], membrane filtration, adsorption [4] and electrochemical treatment. Among them, adsorption is the most efficient, simple, easy and economical method. Recently, several studies have shown that the use of polymers as an adsorbent phase can be an important purification method due to their ability to remove a wide variety of contaminants of different chemical structures and polarity at low concentration. In this context, Chatti et al described the development of a variety of polymers such as poly(ether-pyridine), triazole-based poly(ether-pyridine), polyphosphine and poly(ether-phosphoramide) for high adsorption efficiency of phenolic compounds from water. These polymers were successfully prepared by polycondensation of various fluorinated monomers with two diols, namely isosorbide, derived from renewable raw materials, and bisphenol A, derived from petrochemical products.
The aim of the present work is to carry out a comparative study between the adsorption capacity of petroleum-based and biobased polymers to remove pollutants from water, in order to demonstrate that the incorporation of isosorbide unit into macromolecular chains can be considered an important parameter, which can affect the adsorption efficiency of the resulting polymeric phases.

KEY WORDS: Pollution, water, adsorption, polymers, bisphenol-A, isosorbide, hydrophobic and hydrophilic pollutants.

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The potential of animal and vegetable waste for magnetic extraction of Endocrine Disruptors from water

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Endocrine Disruptors (EDs), including pesticides, pharmaceuticals, and cosmetics, are increasingly detected in environmental waters, raising concerns for human health and ecosystem safety [1]. These endocrine disruptors have been associated with potential risks, such as the alteration of the human endocrine system and possible carcinogenic effects. However, detecting these EDs poses significant challenges due to their low residue levels in real samples and the complexity of the matrices. This study focuses on addressing this challenge by establishing efficient analytical methods for identifying EDs. Specifically, the research emphasizes magnetic solid phase extraction (MSPE), a technique known for its simplicity, speed, and efficiency. To enhance this process, four distinct magnetic adsorbents have been developed utilizing animal and vegetable waste and were characterized using Fourier transform infrared spectroscopy, energy-dispersive X-ray spectroscopy, and scanning electron microscopy. Magnetic extraction parameters were optimized using a Doehlert matrix to determine pesticide and pharmaceutical residues, employing chromatographic methods.

Key words: experimental design, green magnetic adsorbent, Endocrine Disruptors.

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Reversible adsorption efficiency of polyphenols on biobased polymers

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In olive-growing regions, margins constitute a major environmental problem. These residual liquids from olive oil extraction are known to be toxic to flora and fauna, and difficult to biodegrade. Among these polyphenols is this particularly concerning family of compounds: polyphenols, including hydroxytyrosol, tyrosol, caffeic acid and ferrulic acid. Despite their toxicity, these polyphenols are of great commercial value, particularly in the pharmaceutical and agri-food sectors. The main objective of this study is therefore twofold: on the one hand, to reduce the harmful environmental impact of these compounds and, on the other, to exploit their commercial profile by giving them added value. To achieve these objectives, this work has focused on the adsorption technique, which has proved to be the most effective way of removing polyphenols from margins. In this context, we have developed six (06) new polymers (P1-P6) capable of extracting these compounds.

Sorbent regeneration is an important step for certain molecules, such as hydroxytyrosol, which are of interest for their use in cosmetics, and their recovery is of economic interest. In this section, the regeneration of the P6 polymer was studied, as P6 was found to be the most efficient polymer, capable of adsorbing the largest number of target molecules.

Keywords: margins, polyphenols, adsorption, polymers, a precious resource, sorbent regeneration

Application of acetate cellulose electrospun nanofibers on dye removal

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Wastewater treatment is one of the most important means of protecting the water environment from pollution [1]. The abundance of synthetic dyes which is considered as extremely important to treat before it is discharged into the environment. In this study, nanofibers materials are investigated to display a novel approach to improve the properties of materials used in wastewater treatment application. Due to their porosity, large specific surface area and ease of regeneration, electrospun membranes offer a viable material for adsorbing pollutants from aqueous solutions [2]. The elaborated cellulose acetate (CA) nanofibers were used to eliminate dye waste from textile effluents. The obtained nanofibers membranes were characterized using scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FT-IR) and contact angle analysis. The application of elaborated membranes was tested on nanofiltration system since filtration is regarded as one of the most advantageous in dye degradation processes. Therefore, the performance of the CA membranes was evaluated by measuring water flux (PFW) and removal rate for indigo carmine dye using UV- Spectrophotometric method. Experiments were performed as a function of transmembrane pressure and dye concentration. The optimal performances have been obtained at 12 bar of transmembrane pressure and 5 mg/L of indigo carmine concentration. The filtration results showed that the CA membrane elaborated with 48h stirred time was the better membrane in terms of flux (97.30 L/h.m².bar) and of rate of dye removal (83%). These results may be explained by the larger mean pore size and high adsorption capacity recorded. Consequently, the CA nanofibers have a significant potential for removing dye from industrial solutions and can be disposed away in the environment.

Key words: Wastewater treatment, Indigo Carmine, Filtration, Electrospinning, Nanofibers.

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Biochar based electrochemical analysis system for drug micropollutant detection

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Biochar-based materials - which obtained by pyrolysis of renewable biomass resources - have emerged as attractive options for electroanalytical applications due to heir remarkable physicochemical proprieties, including large surface area, strong chemical stability, and good biocompatibility. Their use for electrochemical applications constitutes an emerging approach to satisfy the high demand for micropollutant sensors in environmental samples. Hence, the present work has been devoted to the modification and characterization of a working electrode by biochars doped with different metal particles. The aim is to improve the electrochemical detection of some drug substances such as diethylstilbestrol (DES) which is a non-steroidal estrogen with a high danger to human and environmental health. For this purpose, studies of the electro-oxidation reactions of these substances were carried out on a glassy carbon electrode modified by two copper-based biochars, namely biochar@CuNi and biochar@CuAg. The electrode surface modification was successfully performed and showed significant catalytic activity, especially towards the electro-oxidation of DES with a superiority of biochar@CuAg that showed a significant increase of the current intensity by 97% compared to biochar@CuNi that generated an increase of the order of 19%. This work ends with an initiation of a molecular imprinting polymer (MIP) based polypyrrole development in order to improve the detection selectivity on the surface of the modified electrode.

Removal of antibiotics by adsorption into clay

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This work aimed to study the adsorption of pharmaceutical molecule (Ampicillin) in batch on clay materials. The adsorption isotherms of this molecule were determined in batch at different temperatures on two types of clay: natural and activated by sulfuric acid with modification of the initial concentration of molecule studied from 10 to 100 mg/L. Isotherms obtained were smoothed by Langmuir models, Freundlich and Tempkin. The modeling results show that the Langmuir model perfectly describes the experimental data and gives adsorbed amounts of AMP equal to 48.78 and 86.207 mg/g for natural and activated clay respectively. The study of the effect of temperature (25. 35 and 50 °C) shows that the adsorption process is exothermic and spontaneous.

Key words: Adsorption, kinetics study, equilibrium, ampicillin, activate clay.

Fluorescent Sensors For Detecting Environmentally Toxic Metal Ions

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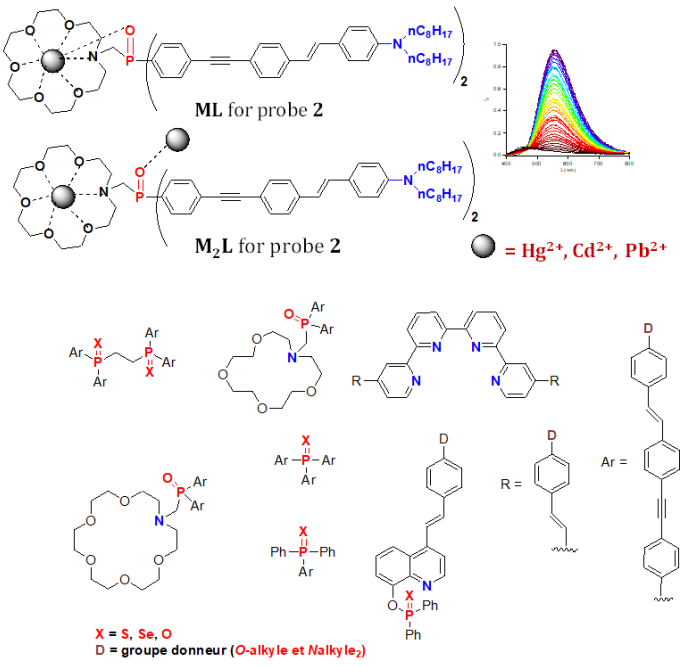
At a time when environmental sciences and the concept of sustainable development are becoming important reference points for our societies, it seems necessary to have the means to fight against pollution. The contamination of water by heavy metals represents an important risk of public health because of the various pathologies that can generate these elements.
In this work, we are interested in the synthesis of fluorescent sensors for the quantification of traces of heavy metals in water.1-4 Three very toxic metallic elements for the environment have attracted our attention: mercury (Hg^{2+}), lead (Pb^{2+}) and cadmium (Cd^{2+}).

Keywords : Probes, sensors, fluorescent environment



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Cost-Effective Additives for High-Performance Laser-Induced Graphene Battery-Like Supercapacitors

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All-solid-state supercapacitors (assSCs) are increasingly demanded for powering small electronics in diverse sectors such as agriculture, healthcare, leisure, and energy grids [1]. Polyimide (PI) is the most used substrate to prepare laser-induced graphene (LIG) for energy storage in assSCs, but they are limited by their specific capacitance which does not exceed 10 $mF \cdot cm^{-2}$ [2]. Our research introduces an innovative and scalable method for step-by-step surface modification of PI-derived LIG electrodes. This approach aims to create highly efficient flexible SCs. We demonstrate that electrochemical modification of the electrode surface using carbon black (CB) particles and redox Berlin blue (BB) significantly enhances the energy storage performance of these supercapacitors. Specifically, the areal capacitance improves drastically: from 12.9 $mF \cdot cm^{-2}$ at 0.1 $mA \cdot cm^{-2}$ for PI-derived SCs to 27.6 $mF \cdot cm^{-2}$ at 0.1 $mA \cdot cm^{-2}$ after CB modification, further escalating to 38.5 $mF \cdot cm^{-2}$ at 0.1 $mA \cdot cm^{-2}$ post BB modification, and reaching 54.4 $mF \cdot cm^{-2}$ at 0.1 $mA \cdot cm^{-2}$ (527.4% increase) for electrodes modified with both CB and PB. Utilizing a H_2SO_4/PVA gel electrolyte expands the electrochemical window to 3.0 V, enabling these modified assSCs to achieve an impressive energy density of 68.04 $\mu Wh \cdot cm^{-2}$ at a power density of 0.3 $mW \cdot cm^{-2}$, measured at 0.10 $mA \cdot cm^{-2}$.

Keywords: Supercapacitors; Additives; Enhancement; Energy storage.

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$ZnFe_2O_4$ nano-composite synthesized through ultrasonic-assisted method for enhanced photocatalytic hydrogen evolution

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Photocatalytic hydrogen production is considered an ideal approach to solving the global energy crisis and environmental pollution. A type II heterojunction photocatalyst, CdS/g-C_3N_4/$ZnFe_2O_4$, was successfully synthesized via the sonication procedure, and it exhibits outstanding photocatalytic performance in hydrogen evolution. The crystal structure, morphology, and electrochemical behavior of all samples were examined by XRD, SEM, HRTEM, XPS, FTIR, UV-Vis, PL, EIS, LSV, photocurrent techniques, Tafel, etc. The corresponding hydrogen production rate of the ternary nanocomposite is 405 µmol g^{-1} under visible light, which is 45.73, 30.04, and 6.46 times higher than that of $ZnFe_2O_4$, g-C_3N_4, and CdS respectively.

Key words: CdS/g-C_3N_4/$ZnFe_2O_4$, photocatalytic hydrogen evolution, charge separation

Improvement of physical properties of ZnO-alloy based for solar cells

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Solar energy is a clean and renewable energy and photovoltaics is one of the most famous energies. Transparent conductive oxide materials (TCO) are important components of photovoltaic (PV) devices that have the greatest impact on solar cell performance. To improve the performance of solar cells, the TCO must have large optical transmission and low resistivity. In addition, high transmission in the visible range and a large band gap of TCO increase the electrical efficiency of photovoltaics. In this work, electrical absorption and transport mechanisms are investigated as key elements for predicting the photoconversion performance of ZnO and ZnO alloy-CdTe solar cells. Using SCAPS-1D software we analyzed the effects of thickness, temperature and doping on the photovoltaic properties: conversion efficiency, form factor, current short circuit and open circuit voltage. The results showed that the small thickness of CdTe was enough to absorb a large amount of light. These results indicate ZnO alloy can be considered as an interesting material to replace CdS window layer.

Keywords: Thin film solar cells, ZnO, SCAPS-1, CdTe thin film,Solar cell performance

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Enhanced electrochemical performance of olive stones-derived activated carbon by aluminum coating for supercapacitor applications

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Porous activated carbon (AC) was successfully elaborated from olive stones and valued as an electrode material for electrical double-layer supercapacitors. The activated carbon surface was subsequently coated by aluminum to improve its physico-chemical and electrochemical properties. The treated activated carbon surface (AC-Al) exhibited a meso-microporous nature. From electrochemical investigations, an improvement of the capacitive behavior was demonstrated after the aluminum coating. Therefore, the activated carbon derived from olive stones and coated by aluminum is a promising electrode material for supercapacitor devices.

Keywords: activated carbon; olive stones; aluminum; supercapacitor.

Investigation of TiO_2 ETM for Perovskite based Solar Cells with Different HTMs

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The Electron Transport Material (ETM) plays a vigorous role on the performance of Perovskite based Solar Cells (PSC). Titanium dioxide (TiO_2) is used as an electron collecting layer. This oxide layer plays an important role. In fact, TiO_2 is the most commonly used material in the semiconductor industry and is considered an alternative to ZnO due to its excellent electron transport.

In this work, TiO_2 ETM is analyzed with diverse Hole transport materials (HTMs). Spiro-OMeTAD, PEDOT:Pss, and Cu_2O are suggested for lead-free $CH_3NH_3SnI_3$ based Perovskite solar cells. The influence of device parameters such as thickness of the active layer, doping level of the $CH_3NH_3SnI_3$ layer and working temperature is discussed for optimum parameters of all structures (efficiency, V_{CO}, I_{cc}, FF). It has been shown that efficiency can be upgraded if TiO_2 is used as ETM layer, and the cost can be reduced.

Key words: Perovskite, TiO_2, ETM, Simulation, SCAPS-1D software.

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Physico-chemical characterization, Hirshfeld surface analysis and DFT calculation of a hybrid material: 4-(2- ammonioethyl) morpholin-4-ium dichloridodiiodidocadmate/chloridotriiodidocadmate

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The crystal structure of partial substituted compound 4-(2- ammonioethyl) morpholin-4-ium dichloridodiiodidocadmate/chloridotriiodidocadmate (0.90/0.10) as monoclinic $P2_1/c$, with $a = 6.7773(14)\text{Å}$, $b = 13.870(3)\text{Å}$, $c = 16.104(3)\text{Å}$; $V = 1510.5(5)\text{Å}^3$. Single-crystal X-ray diffraction analysis indicates that the asymmetric unit in this compound consists by one-dimensional (1D) cationic chain $[NH_3(CH_2)_2NH(CH_2)_4O]^{2+}$ linked via N-H…O hydrogen bonds extending parallel to the c axis and an isolated $[CdCl_{1.90}I_{2.10}]^{2-}$ tetrahalidocadmate anions; which are interconnected via N-H… Cl and C-H…Cl(I) hydrogen ensuring the formation of a three-dimensional (3D) network. Infrared spectroscopy confirms the presence of the organic moiety in the structure. Hirshfeld surface analysis has been performed to investigate the intermolecular interactions and crystal packing of the title compound. Optical properties were recorded at room temperature using UV-visible spectroscopy in the spectral range 200-700 nm. The electronic transition of the title complex was recorded in ethanol solvent and the electronic distribution of HOMO − LUMO was rationalized theoretically through density functional theory (DFT).

Keywords: Organic-inorganic hybrid material; Single crystal X-ray diffraction; Crystal structure; Hirshfeld surface, DFT calculation, Vibrational study, Optical absorption.

Radiation-Induced Modification of LDPE: Effects of Electron Beam Accelerator Exposure

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Radiation is currently being exploited to modify polymers in order to improve properties for various applications. This paper thoroughly examines the effects of high energy electron beam irradiation (10 MeV) on low density polyethylene (LDPE) material. LDPE was subjected to a broad range of doses ranging between 10 and 300 kGy at room temperature under different conditions. Extensive characterization techniques such as the Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC) were conducted on the non-irradiated and irradiated samples. Our findings revealed significant changes in LDPE's chemical structure after irradiation under air atmosphere by the formation of carbonyl groups located at 1715 cm^{-1} proving its oxidation degradation. The determination of carbonyl index showed that the irradiation effect was more noticeable when higher levels of irradiation were applied. In addition, the evaluation of the mechanical properties of LDPE in terms of tensile strength and elongation at break showed that these properties were significantly affected independently of the irradiation conditions. Finally, this research sheds light on the complex interplay between irradiation conditions and LDPE's structural properties, offering valuable insights for applications in polymer materials and radiation-induced modifications.

Keywords

High-energy radiation, LDPE, carbonyl index, mechanical properties.

A new 0-D hybrid bismuth halide compound $(C_{13}H_{28}N_2)_4$ $[BiCl_6]_2$ .2Cl. 5 H_2O: Synthesis, crystal structure and physical properties

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Zero dimensional (0-D) hybrid bismuth halide materials have aroused high interest due to their hopeful emission properties [1-2]. Here, we report the synthesis by slow evaporation method and the characterization by single-crystal X-ray diffraction (SC-XRD), thermal analysis and optical measurements of a novel hybrid material 0-D $(C_{13}H_{28}N_2)_4[BiCl_6]_2.2Cl.5H_2O$. The structure of the title compound was determined by single-crystal X-ray diffraction (SC-XRD) at 296 K. Crystal data: Orthorhombic crystal system, space group Pna21, a = 6.587(2) Å, b = 11.697(4) Å, c = 14.625(5) Å, α = 90°, β = 92.514(6)°, γ = 90° and V = 2662.5(9) Å3 . The asymmetric unit of the structure contains four 4,4'-methylenebis(cyclohexylammonium) organic cations, two hexachlorobismuthate anions, two chlorine atoms and five water molecules. The crystal packing of the obtained compound is governed by the formation of various non-covalent intermolecular forces (H-bonding, Coulomb interactions, Van der Waals interactions) between BiCl6 3- anions and organic cations, assisted by water molecules. Hirshfeld surface analysis denotes that the most important contributions to the crystal packing are Cl···H/H···Cl and H···H interactions. The DSC/TGA curves presents two bands at 79 °C and 200 °C attributed to dehydration and to the decomposition of the material respectively. The diffuse reflectivity of powder sample was measured to obtain the band gap energy (Eg). The Eg of compound is calculated by the Kubelka-Munk method to be 3.36 eV, indicating that the compound can be classified as a semi-conductor. The photoluminescence analysis indicates that compound emits the strong yellow-orange light at 639 nm, which should be attributed to the charge transfer between Bi3+ and Cl- .

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Upconversion luminescence for temperature sensing in Er^{3+} doped phosphate materials

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In the pursuit of highly precise thermometry, the development of effective optical temperature sensors becomes increasingly significant. This study centers on the comparison of two materials, Mg3P:Er^{3+} and Mg2P:Er^{3+}, with a specific focus on their potential as novel, precise thermometers. The investigation delves into the fundamental physicochemical properties of the synthesized materials, encompassing aspects such as crystal structure, morphology, upconversion (UC) emission, and temperature dependence. The UC luminescence properties of the micro-sized particles synthesized are explored across a broad temperature range, spanning from 303 to 473 K. Temporal evolution studies offer confirmation that excited state absorption is the fundamental mechanism of the observed upconversion emissions. Temperature sensing study demonstrates different relative sensitivities in both materials. Our findings establish that Mg2P:Er^{3+} displaying the highest relative sensitivity in temperature sensing, albeit with a slightly increased error margin.

KEYWORDS: Phosphate materials; luminescence; lanthanides, upconversion emission; Temperature sensing,

Integration of efficient single photon sources by plasmonic enhanced two-photon polymerization of multifunctional photopolymers

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The integration of nano-emitters into plasmonic and photonic devices with spatial control and nanometer precision has become a great challenge. In this work, we report on the use of a hybrid and functionalized photopolymers [1, 2] to selectively integrate nano-emitters on specific preselected sites of plasmonic nano-antennas and optical waveguides. For this, two approaches were developed to integrate the nano-emitters (See Figure 1).

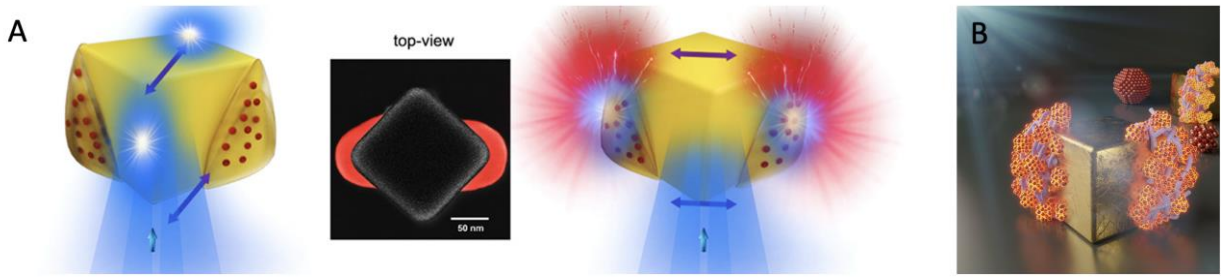

Figure 1: Figure illustrating our integration approaches for the creation of efficient photon sources. A: integration of QDs in a spatially controlled manner by local near field TPP of a QDs-containing photopolymer in the vicinity of a single gold nanocube. B: fabrication of a hybrid photon source after integration of a smart functionalized polymer by local near field TPP and electrostatic immobilization of QDs.

The first one consists of using a photosensitive formulation containing quantum dots (QDs) where acrylic monomers are grated on Blue, Green and Red emitting QDs. This hybrid photopolymer is then used to integrate the nano-emitters by 2-photon polymerization (TPP) in the near field of a single gold nano-cube [3, 4]. The second approach uses functionalized photopolymers making it possible to attach negatively charged nanoparticles right at the preselected polymerized sites, which subsequently recognize the nano-emitters to be attached [2]. Since the resulting active medium is a spatial memory of specific plasmonic modes, it is anisotropic, making the hybrid nanosources sensitive to light polarization [4, 5]. The ability to adjust their statistical average lifetime by controlling the volume of the nanopolymer is demonstrated on two kinds of nano-emitters coupled to GNCs: doped polystyrene nanospheres and semiconductor colloidal quantum dots. These 2 approaches have been investigagted to integrated single photons sources in a specially controlled manner into photonic and plasmonic nanostructures.

Key words: Quantum dots, single photon sources, plasmonic nanoantennas, Two photon polymerization, Photopolymers, polymer surface functionalization, Quantum technologies.

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Elaboration of new objects belonging to coordination chemistry and molecular magnetism

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The field of molecular magnetic materials is strongly evolving and one of the most challenging areas of functional materials science.

The ability of some discrete paramagnetic polynuclear clusters to exhibit hysteretic properties below a certain temperature leads to its classification as **S**ingle-**M**olecule **M**agnets (**SMM)**. Combination of the properties typically associated with conventional magnets with molecular distinctive properties as small size, solubility in organic solvents, highly crystalline structure, low density, transparency and low-temperature fabrication offer a wide field of applications including fundamentally different way to process and to store information, such as quantum-based computing.

The important factors in the construction of SSM derive from the combination of a large value of the ground spin state and a large magnetic anisotropy of the Ising (easy-axis) type. The main challenge here is to assemble in a controlled manner several magnetic centers in one molecule (cluster) isolated from the neighbors.

The chemical approach of our investigations was based on the use of new high-bulky organic ligands containing the different types of donor atoms.

In this presentation we will talk about the synthesis, crystal structure and magnetic properties of several new polynuclear complexes with 3d-elements.

Keywords: schiff base ligands; magnetic properties; polynuclear complexes; simulation.

Elaboration, structural study and biological activity of a new cadmium complex

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The elaboration and development of innovative multifunctional complexes represent a cross-disciplinary research area. This is not only because of their fascinating structures and diverse forms but also due to their wide-ranging uses in catalysis, magnetism, optoelectronics, biological and medical sciences [1]. In this context we have focused our work on the synthesis of an unreported cadmium complex of formula $[Cd(NO_3)_2(C_6H_7NO)_4]$. This compound crystallizes in the monoclinic $P2_1/c$ space group with a = 11.040(2) Å, b = 9.152(2) Å, c = 14.694(3) Å and β= 107.63(2). The resolution of the structure leads after several cycles of refinement followed by some Fourier-Differences to reliability factors R (F) = 3.09% and wR (F2) = 8.92%. The central cadmium ion is coordinated by four O atoms from 6-methyl-2-pyridone ligands and by two O atoms from two nitrate anions ligands, in a distorted octahedral coordination environment.

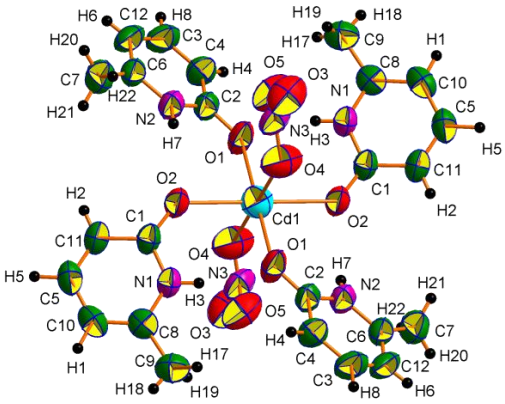

Figure 1: Asymmetric unit of $[Cd(NO_3)_2(C_6H_7NO)_4]$

The formed layers are interconnected to the framework through π-π stacking interactions between the 6-methyl-2-pyridone ring systems of adjacent ligands. The cadmium complex underwent characterization through techniques such as IR spectroscopy and thermogravimetric analysis. In vitro testing was conducted to assess the antibacterial activity of the synthesized complex against both Gram-negative and Gram-positive bacteria, confirming its biological efficacy.

Key words: Cadmium complex, structural study, TG analysis, biological activity

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Synthesis, Structural and spectroscopic studies, thermal characterization and Hirshfeld surface analysis of Cobalt (II) complex $[Co(C_6H_6N_2O)_2(H_2O)_4](NO_3)_2.2H_2O$

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In this work, a new cobalt hybrid compound $[Co(C_6H_6N_2O)_2(H_2O)_4](NO_3)_2.2H_2O$ was synthesized as single crystals by slow evaporation at room temperature. The physico-chemical characterizations of the prepared compound were done by various experimental techniques: powder and single crystal X-ray diffraction, spectroscopic studies (IR and UV-visible) and thermal analysis (TG).

The single crystal X-ray diffraction study showed that the compound crystallizes in the orthorhombic system with the space group Pbca. The final values of the veracity factors are: R1= 0,026 for 3133 reflections, wR2 = 0.105 and S = 0.85. The asymmetric unit of the studied compound consists of a complex cation $[Co(C_6H_6N_2O)_2(H_2O)_4]^{2+}$, two NO_3^- anions and two molecules of water of hydration. The structural arrangement of $[Co(C_6H_6N_2O)_2(H_2O)_4](NO_3)_2.2H_2O$ shows a succession of alternating organic/inorganic chains propagating along the a-axis interconnected via N-H...O and O-H...O hydrogen bonds and π-π interactions giving the structure its cohesion and stability in a three-dimensional network. Thermal analysis was performed to display the different steps of weight loss relative to the title compound. The analysis of the Hirshfeld surfaces (d_{norm} and shape index) associated to 2D fingerprint plots has been done in order to strengthen and consolidate the study of the elaborated complex it helped quantifying the relative contributions of the inter-molecular interactions in the crystal structure.

Key words: hybrid compound, single crystal, Hirshfeld surfaces, thermal analysis.

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A novel ionic– protonic conductor compound based on tellurium: Synthesis, crystal structure, thermal behavior, Hirshfeld surface analysis, electric and vibrational properties

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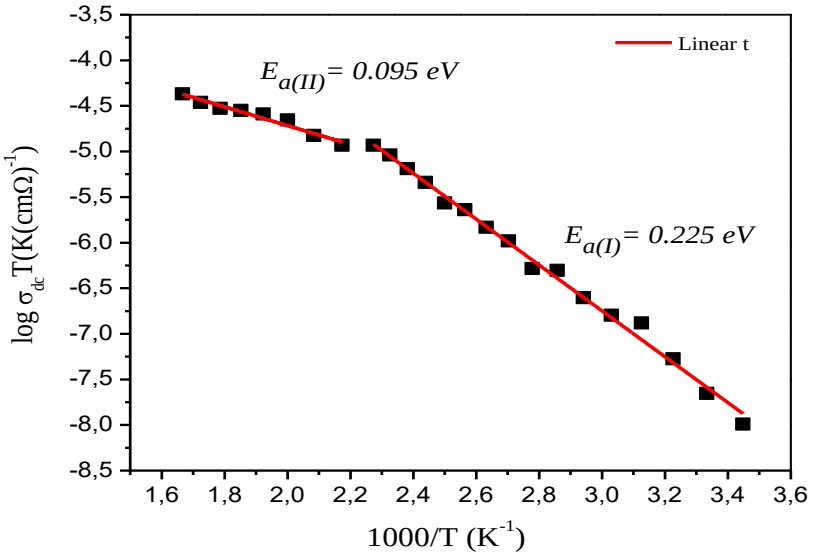
In the current research work, we investigated the growth of the new potassium arsenate tellurate material formulated as $K_3(HAsO_4)(H_2AsO_4).Te(OH)_6$(KAsTe) through the use of the hydrothermal preparation method. The KAsTe compound was crystallized in the monoclinic system with centrosymmetric space group *C*2/*c*. Within this structure, two types of polyhedra (TeO_6 and $HAsO_4$) were observed in the presence of K^+ cations. The stability and the cohesion of the crystal structure were ensured by the linkage of different polyhedra via O–H···O hydrogen bonds. Thermal analyses (DSC, DTA, TG and MS) proved the presence of three phase transitions at 428, 510 and 553 K and indicated that no mass loss was recorded before 460 K. Furthermore, the σ_{dc} variation performed on KAsTe material suggested an important level of conductivity at high temperature, associated with the motion of H^+ proton. This behavior goes in good agreement with the presence of the super–ionic protonic phase transition at 428 K.



Temperature dependence of (log (σT)) for KAsTe compound.

Sol-gel derived (Zn–)TiO_2 for ultraviolet transmittance: Effect of the surfactant nature on the morphological and structural properties

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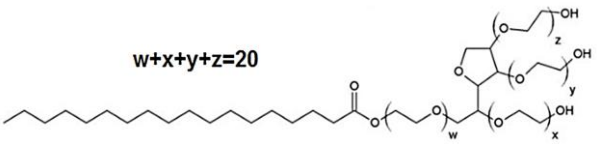
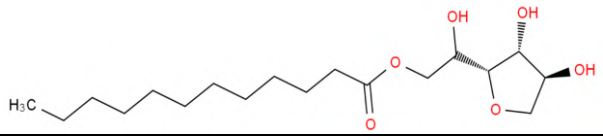
TiO_2 and ZnO have been used for decades in the formulation of sunscreen lotions in order to avoid the harmful effects of sun. Effectively, the exposure to ultraviolet (UV) radiation can lead to several damages, namely for patients suffering from *xeroderma pidementosum*.
Sol–gel method is one of the well-establish route for the preparation of (Zn–)Ti oxide with controlled texture and morphologiy. The aim of this study is the preparation of (Zn–)TiO_2 with minimum UV transmittance by sol-gel method after varying the nature of surfactant. Starting from titanium alkoxide alcoholic solution, the surfactant was added in the appropriate amount before adding HNO_3 for hydrolysis. The gel is then dried in oven before being treated under air at a particular temperature and for appropriate duration. According to X-ray diffraction, no rutile polymorph was detected, and the size of particles (determined by *Scherrer* formula) is less than 15 nm. Table 1 illustrates the maximum transmittance values obtained in the 200–400 nm wavelength range.

Table 1: The maximum percent transmittance obtained between 200 and 400 nm for different titania samples (1 mg mL^{-1}) issued from different surfactant.

Surfactant	Chemical structure	Transmittance
Tween 80		69 %
Tween 60 *2-{2-[3,4-bis(2-hydroxyethoxy)oxolan-2-yl]-2-(2-hydroxyethoxy)ethoxy}ethyl dodecanoate*		79 %
Montane 60 *(2R)-2-[(2R, 3R, 4S)-3,4-dihydroxyoxolan-2-yl]-2-hydroxyethyl dodecanoate*		0 %
Montanov 68		46 %

According to Table 1, the transmittance of titania nanoparticles depended on the chemical structure and the size of surfactant molecule. For the sample issued from Montane 60, the scanning electron microscopy excluded the agglomeration of particles upon calcination. Additionally, the obtained results indicate that the morphological and structural properties of TiO_2 and Zn-TiO_2 issued from Montane 60 are similar, which is encouraging to give more insight into the formulation of sunscreen lotion.

Keywords: Sol-gel, TiO_2, transmittance.

THE RELEVANCE OF CATALYTIC SILICATE AND CARBON DUST SURFACE REACTIONS IN THE INNER SOLAR NEBULA

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We live in a dusty Universe! Dust is not only found in our solar system among the planets, but it is present in a wide variety of objects throughout the Universe, mainly in those regions between stars called interstellar clouds. The interstellar medium particles -generally composed of an intimate mixture of silicate and carbon grains- and the interstellar gas are perpetually interacting. The aim of our study is to understand the dynamics of this interaction between the matter in the gas phase and the nanoparticles in new physical conditions and see how this influences the chemical complexity of space, particularly on the formation of planets. A coherent and interdisciplinary approach is required to quantify the active and catalytic role of dust in space [1].

First of all, we will produce in the laboratory dust particles analogous to the silicate dust observed in the interstellar medium. Then, we will perform experiments to study the reactions on the surface of the dust grains under astrophysical conditions and characterize the obtained products using the techniques: X-Ray Photoelectron Spectroscopy (XPS). Finally, we will exploit the results of our study to define relevant astrophysical environments using a molecular dynamic simulation and develop additional modules for these simulations that describe the new dust functionality.

Key words: Interstellar grains, interstellar gas, catalytic role, molecular dynamic simulation.

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Physicochemical Characterization and Electro-conductivity of Novel Zirconium Oxide-Crystalline Cerium(iv) Phosphate/ Polybenzimidazole-co-Polyaniline, co-Polyindole, co-Polycarbazole Nanocomposites

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Crystalline cerium (iv) hydrogen phosphate $Ce(HPO_4)_2.1.33H_2O$(CeP), and nano particles zirconium oxide($nZrO_2$), of average size 19.3nm, were prepared and characterized by chemical, XRD, FT-IR and TGA analysis. Mixing slurry aqueous solution of $nZrO_2$ and CeP in 25:75 wt/wt% mixing ratios, respectively, lead to formation of novel zirconium oxide-cerium phosphate nanocomposite, $[ZrO_2]_{0.25}$ $[Ce(HPO_4)_2]_{0.75}.1.33H_2O$($nZrO_2$-CeP). $[nZrO_2]_{0.25}[CeP]_{0.75}$/polybenzimidazole-co-polyaniline, co-polyindole, co-polycarbazole nanocomposites, were prepared via in-situ chemical oxidation of their parent-co-monomers. A possible explanation is part of CeP, of inorganic composite ($nZrO_2$-nCeP) is attacked by the parent co- monomers converted to cerium(III) orthophosphate($CePO_4$). The resultant nano composites. ere characterized by elemental (C, H, N) analysis, FT-IR, UV-Vis and scanning electron microscopy(SEM). From elemental (C, H, N) analysis the amount of % in wt. of organic materials present in ($nZrO_2$-CeP)/polybenzimidazole copolymers nanocomposites were for PBI-co-Pani [PBI=8.59%, Pani=11.53%], for PBI-co-PIn [PBI=8.33%, PIn=14.83%], for PBI-co-PCz [PBI=10.94%., PCz=15.51%. Electrical conductivity of resultant copolymers nanocomposites was investigated using DMSO solvent, found to be $2.13x10^{-6}$, $3.02x10^{-6}$ and $2.53x10^{-6}$ S/cm, respectively, represent range of semiconductors.

Keywords: nano zirconium oxide, crystalline cerium phosphate, polybenzimidazole -co-polyaniline, co-polyindole, co-polycarbazol, nanocomposites, electrical conductance.

Comparison between the antitumor activity of decavanadate compounds

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Decavanadates have been widely investigated because of their many interesting properties and their potential use in several applications. In this work, we compare the antitumor activity of three decavanadate compounds: $(C_4N_2H_7)_4(C_6N_2H_{10})V_{10}O_{28}\cdot 2H_2O$ (**CI**), $Mg(H_2O)_6(C_4N_2H_7)4V_{10}O_{28}\cdot 4H_2O$ (**CII**) and $(C_4NH_{10})_4(H_2V_{10}O_{28})\cdot 2H_2O$ (**CIII**) against three invasive cancer cell lines; U87 (glioblastoma), IGR39 (melanoma) and MDA-MB-231 (triple negative breast cancer). Thus, the presented work show a great potential of decavanadate compounds to be developed into novel anticancer agents applicable also in the malignant cells resistant to the current conventional drugs.

Keywords: Decavanadate, Antitumor activity, U87, IGR39, MDA-MB-231.

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PREPARATION AND ANALYSIS OF BIOCHAR-ZNO CATALYST FOR ELECTROCHEMICAL DEGRADATION OF CONGO RED IN WASTEWATER

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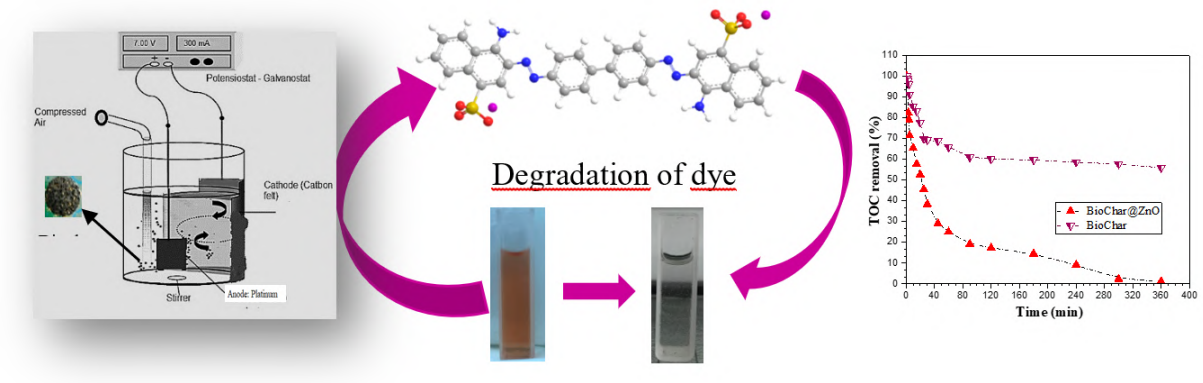
In this study, we initially outlined the process of converting agricultural biomass waste (Moringa Oleifera) into active biochar. The catalyst precursor was a mixture of Moringa Oleifera biomass powder and zinc acetate salt. This mixture underwent pyrolysis at 500°C in an inert environment, resulting in the uniform dispersion of ZnO nanoparticles on the biochar surface. We characterized the composite materials using various techniques, including XPS, Raman spectroscopy, FESEM (Field Emission Scanning Electron Microscopy), and XRD (X-ray Diffraction). The primary focus of our investigation was the electrochemical degradation of Congo Red (CR). The electrochemical reactor consisted of two-cell electrodes: a platinum anode and a carbon felt cathode, facilitating the generation of H2O2 through the reduction of O2. Utilizing biochar-ZnO as a heterogeneous catalyst in the discoloration of CR via an electrochemical process proved to be highly effective. It led to the near-complete mineralization of the CR solution, with over 98% removal of total organic carbon achieved after approximately 300 minutes.

Graphical abstract



Theoretical and experimental characterizations of a hybrid compound based on peprchlorate salts

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The slow evaporation approach was used to create the hybrid compound (C5H8N3)ClO4 in aqueous solution at room temperature. It crystallizes in the monoclinic non-symmetric space group P21 with the parameters a=5.1261 (9), b=9.3003 (17), c=8.6659 (16), and = 102.595 (7)°. The supramolecular crystal structure, on the other hand, was composed of perchlorate anions (ClO4)- and organic diaminopyridinum cations (C5H8N3)+ linked together by hydrogen bonds to form a three-dimensional network. The vibrational modes relate to both inorganic and organic species, according to the Fourier transform infrared (FTIR) and Raman spectra. According to Hirshfeld's study, the existence of hydrogen bonding O...H (50% of the time) stabilizes the crystal packing.

A new halide hybrid compound based on Cu (II) and 2-amino-4-picoline: A combined experimental and theoretical study.

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Organic-inorganic hybrid materials represent an exceptional class of materials that synergistically combine the characteristic physical properties of organic and inorganic components, particularly mononuclear hybrid perovskites. Chemistry has led to the emergence of numerous new hybrids with very diverse applications, particularly medical and cosmetic applications, photovoltaics **[1]**, catalysis **[2]**, biocatalysis and separation biocatalysis **[3]**. We have successfully synthesized a novel organic-inorganic hybrid compound which possesses required crystallographic, thermal and optical properties. This complex $(C_6H_9N_2)[CuCl_4]$ was characterized by single crystal X-ray diffraction (XRD), thermal studies, IR and UV-Vis spectroscopy. The compound crystallizes in the C2/c monoclinic space group system. Moreover, the optimized molecular structures and vibration frequencies were calculated by density functional theory (DFT) using the B3LYP function with the LanL2DZ basis set. The bond lengths and angles obtained from the structural analysis agree well with the theoretical ones obtained from DFT. To confirm the results obtained by X-ray diffraction, infrared spectroscopic measurements were carried out. Furthermore, the strong absorption of the UV region is explained by the optical properties of the studied Cu hybrid. Thermal analysis tests were also carried out, which revealed the occurrence of phase transitions in the temperature range from room temperature to 600 °C.

Key words: Organic template; Metal halides; DFT calculations and Vibrational frequencies.

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Polyol Synthesis of Copper doped Gold@ZnO Nanorods for the Degradation of Diuron with Solar Light in Liquid Phase

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In the present investigation, Copper-doped Au@ZnO nanorods ($Au@Zn_{1-z}Cu_zO$) were synthesized using a one-pot polyol method, incorporating a low Cu molar content ($0 < z < 1\%$). These nanorods were then assessed for their effectiveness in the photodegradation of Diuron, which is among the most environmentally harmful and persistent herbicides found in aquatic ecosystems. The polyol solvent, triethylene-glycol (TREG), played a crucial role as both a reducing agent and a stabilizing agent, influencing the morphology, size, and photocatalytic properties of the $Au@Zn_{1-z}Cu_zO$ photocatalysts. The structural and morphological characteristics of the synthesized nanoparticles were analyzed using X-ray diffraction (XRD), transmission electron microscopy (TEM), energy dispersive X-ray spectrometry (EDX), UV-Vis diffuse reflectance spectroscopy (DRS), and nitrogen adsorption (BET). These $Au@Zn_{1-z}Cu_zO$ nanorods, with an optimized Cu content of $z = 0.1\%$, exhibited photocatalytic activities approximately twice as high as undoped Au-ZnO nanorods under solar light irradiation. This enhancement is attributed to the superior charge separation rates observed in the $Au@Zn_{1-z}Cu_zO$ nanorod structure.

Keywords: Copper doped Au@ZnO nanoparticles; Triethylene-glycol; Photocatalytic activity; Diuron.

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$Cu_3(BTC)_2$ hybrid material via conversion of copper (II) hydroxide: Synthesis and caracterization

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Metal-organic frameworks (MOFs) are a class of crystalline hybrid materials prepared via well-established principles of coordination chemistry using the self-assembly of metal ions or oxo-metallic clusters with organic linkers [1]. The growth of thin continuous films of MOFs on different substrate surfaces has been identified as a pressing research challenge. Indeed, the use of these materials for technological application and devices elaboration, such as sensors, requires their interfacing to two or three- dimensional substrate either in the growth stage or within the device itself [2]. In this work, the fabrication of MOFs thin films has been achieved by different methods including layer-by-layer deposition. In this work, we describe a simple and straightforward methodology based on the in situ conversion of copper hydroxides to $Cu_3(BTC)_2$ thin films on glass substrate using the layer by layer growth method. The obtained product was characterized by ATR-FTIR, X-ray diffraction (XRD) and, optical and scanning electron microscopy.

Key words : Copper hydroxide, MOFs, SURMOF, Cu3(BTC)2

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Synthesis and characterization of calix[4]arene diester-grafted functionalized clay nanocomposites

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The present work studied the synthesis of nanocomposites calix[4]arene-modified-clay. The calix[4]arene diester was prepared and characterized. Purified clay was firstly silylated with APTES silane before grafting the glutaraldehyde. Then, tris(2-aminoethyl)amine, ethylenediamine or hexamethylenediamine were grafted. The structures of the silylated and modified clays were characterized by various techniques. The calix[4]arene diester was grafted onto modified clays. All data demonstrated the successful grafting of calix[4]arene, and indicated that in the case of the nanocomposites with aliphatic amines, the calixarene was grafted by a single ester function, whereas by two ester functions in the case of the nanocomposite with branched amine.

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Nanotechnology a promising tool in pharmaceutical industry

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These recent years nanotechnology has shown as a promising concept in various medical and healthcare fields especially in pharmaceutical industry.

Scientist researches have demonstrated that this innovative technology enables better construction and advanced product design and increases quality, efficacy and safety of pharmaceutical preparations.

In this communication we will understand the influence of nanoparticules chemical characteristics on the stability and bioavailability of pharmaceutical formulations so their therapeutic effect.

We will highlight the current progress in complicated disease therapies in correlation with the issues of nanoparticules engineering technologies by giving some examples of the innovative applications for nanotechnology in pharmaceutical industry.

Then we will discuss the possibilities and challenges of developing such innovative and promising therapies which created a huge gap between scientific researches and market access.

Key words: Nanotechnology, pharmaceutical industry, stability, bioavailability, market access.

Design and Synthesis of Highly Sensitive Fluorophores for Heavy Metal detection

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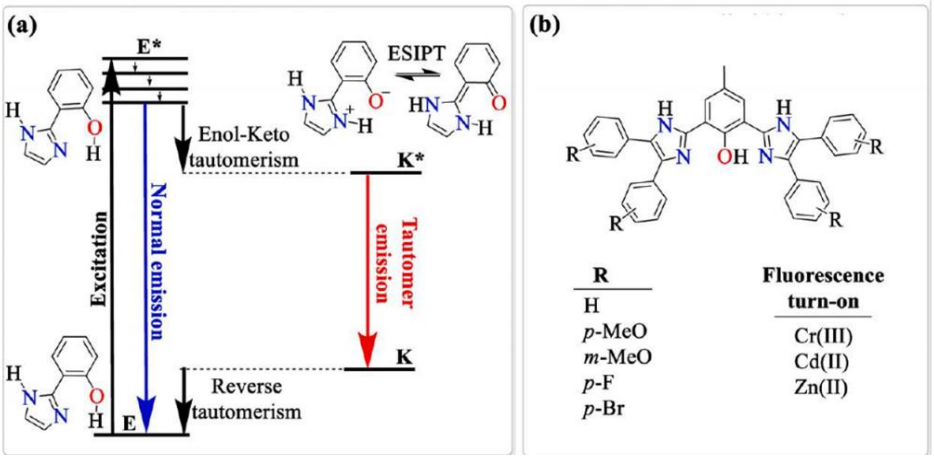
Novel chemosensors with diverse electronic properties and conjugation patterns, specifically designed for Mercury detection**[1, 2]**. Through mercury titration and X-ray structural data, the results reveals a 1:2 interaction ratio between these ligands and Hg^{2+} ions. Additionally, structural analysis identifies the loss of fluorescence in these sensors, attributed to the twisting of aromatic rings in the central imidazole-phenyl-imidazole structures, disrupting their core π-conjugation.

In summary, this work contributes to the development of highly precise and sensitive molecular sensors for heavy metal detection, employing innovative ESIPT-based dyes and customized bis-imidazole-phenol fluorophores.



Scheme 1. (a) Illustration of the ESIPT process, which leads to red-shifted emission,

(b) bis-imidazole molecules previously studied

Key words: Bimidazole, Chemosensors, fluorescence, ESPIT, Heavy metal detection, X-Ray

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Coumarins hybridization of Zn (II)-Montmorillonite for enhanced fluorescent Materials: Spectral and Structural characterization

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New coumarin derivatives (methylphenyl, chlorophenyl and nitrophenyl named respectively C1, C2 and C3), have been prepared according to Mhiri et al. [1] and characterized via H^1NMR, FT-IR, UV-vis and Fluorescence spectroscopy. C1 and C2 showed intense blue fluorescence when excited at 325 nm while C3 emitted a weakly blue light. Their binding properties towards transition metal cations and some lanthanides have been studied by UV-visible absorption. Complexes ML_2 (M: metal; L: coumarin) have been formed upon titration with metal cations. The chelating of C1-C3 induces a change in luminescence properties of C1-C3.

We also highlight recent advances in the development of coumarin-based clay hybrids. A green reaction between Zn (II) exchanged montmorillonite (ZnMMT) and C1-C3 have been established. The spectral and structural characterizations of the new hybrids (C1ZnMMT, C2ZnMMT and C3ZnMMT) have been established by XRD and FTIR. The adsorption study of coumarins by ZnMMT has shown that complexes of Zn^{2+} have been formed into the interlayer space of montmorillonite. In order to assess their potential suitability as chemical sensors, their luminescent properties have been investigated.

Keywords: Coumarin, Complexes, Zn (II)-Montmorillonite, Hybrid, Fluorescence.

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Characterization of Nanostructured Tantalum Carbide Synthesized by Mechanical Alloying

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Tantalum carbide (TaC) is a candidate material for high-temperature use, such as that required for high-performance cutting tools and aerospace propulsion systems, because of its high melting point (>3800 °C), high elastic modulus (537 GPa), high Vickers hardness (>9.4 GPa), and superior thermal and chemical stability. In this work, titanium carbide nanopowders (n-TaC) were produced by mechanical alloying (MA) through high-energy ball milling from a mixture of elemental powders of tantalum (Ta) and graphite (C) in argon atmosphere. MA process was performed for 20 h using a planetary ball mill at a ball-to-powder weight ratio of 70:1. Microstructure and morphology of the samples were studied by X-ray diffraction (XRD), laser granulometry, and scanning electron microscopy (SEM). XRD studies revealed that in the times more than 15 h of MA all the raw materials were changed to the desired materials. Results showed that nanocrystalline TaC, with about 11 nm, is synthetized by reaction between Ta and C atoms.

Key words: Mechanical alloying, Nanostructure, TaC, Microstructure

Polydopamine modified laser-induced graphene electrodes for capacitive sensing of nitrites ions

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Nitrite is commonly present in both the natural environment and human activities; however, its misuse and potential harmful effects pose a significant risk to human health [1]. Hence, accurate detection of low levels of nitrite is of utmost importance for maintaining the quality of drinking water and food products. The use of graphene-based materials for electrochemical sensing of these ions have been regarded as one of the most promising detection tools due to their high sensitivity, simplicity of operation, and excellent selectivity [2-3].

In this context, we developed laser-induced graphene electrodes (LIGEs), by laser ablation of a polyimide substrate, subsequently modified by electrochemical deposition of polydopamine film (PDA/LIGE). Electrochemical measurements were conducted to assess the physico-chemical properties, including laser-induced porous graphene features, such as the heterogeneous electron transfer (HET) rate and the electrochemically active surface area (ECSA). Furthermore, taking advantages of the redox activity of PDA film, we studied the potential of redox capacitance spectroscopy as a sensitive and highly adaptable nitrite ion sensing methodology. Upon nitrite interaction with PDA/LIGE electroactive interface, the redox distribution and its associated redox capacitance are altered, which allowed the successful detection of nitrite ions with a linear response, ranging from 10 µM to 10 mM, and a limit of detection of 2.45 µM. Moreover, we applied the developed sensor to analyze nitrite levels in tap water and mineral water, yielding good recoveries. These results demonstrate the potential of our approach as a promising method for routine detection of ions.

Key words: Laser-induced Graphene, Polydopamine, Capacitive detection, Sensor, Nitrite.

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Geometrical and relative stabilities of iron oxide clusters Fe_nO_m

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Encouraged by the use of Fe_2O_3 nanoparticles for treating cancer, we have explored the structural features of these particles [1]. Our research concentrated on $(Fe_2O_3)_n$ as a model system, enabling the physisorption of oxygen atoms on the surface of the respective unary Fe_n cluster when n ranges from 1 to 100. The geometric properties of iron oxide clusters $(Fe_2O_3)_n$ are theoretically investigated using the Monte Carlo (MC) optimizations technique. This method is founded on both the potential model (PM) and the Basin-Hopping (BH) approaches [2,3]. In this present work, we have developed a novel algorithm/program to investigate all metal oxide clusters $(M_xO_y)_n$. The total potential energy V of the studied systems is written as the sum of the O-O, Fe-Fe, and Fe-O interactions. An empirical many-body potential is used to develop a potential model allowing an accurate description of the binding energy of $(Fe_2O_3)_n$ nanoparticles [4-6]. The stable clusters are obtained by exploring the potential energy surface of the Fe_2O_3 molecule. Comparisons with available theoretical and experimental data show good agreement, which is a good examination of the reliability of our theoretical method [7-9].

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Fe-based alloys produced by mechanical milling: Structural and thermal characteristics

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Nanocrystalline FeCoNi and FeCoNiSi powdered alloys were prepared by mechanical milling process (MA). Indeed, using X-ray diffraction patterns, we experimentally proved that when MA reached a time of 50h, it led to a decrease of the crystallite size down to 20 nm and 32 nm for FeCoNiSi and FeCoNi respectively. However, the dislocation density increased reaching the highest value for the alloy associated to silicon. Nevertheless, this high energy ball-milling process is not used only for the refining of microstructure, but also to induce either a chemical reactions between the powdered chemical elements or a phase transformations, such as the allotropic transformation of HCP-Co to FCC-Co and the formation of highly disordered Fe-based solid solutions. Thermal stability of the milled mixtures was investigated by DSC from 25 up to 700°C at a heating rate of 10°C/min. Besides, various of the milled samples were first annealed at specific temperatures and then analyzed using X-ray diffraction, which demonstrated the stability of the evolved phases during subsequent heating and the formation of some metallic oxides, such as Fe_3O_4, Fe_2O_3 and FeO, particularly for the elevated annealing temperatures

Key words: Milling; Nanostructures materials; annealing, DSC; X-ray diffraction.

Synthesis and characterization of α,α'-diimine ligands: A new precursor for novel coordination complexes

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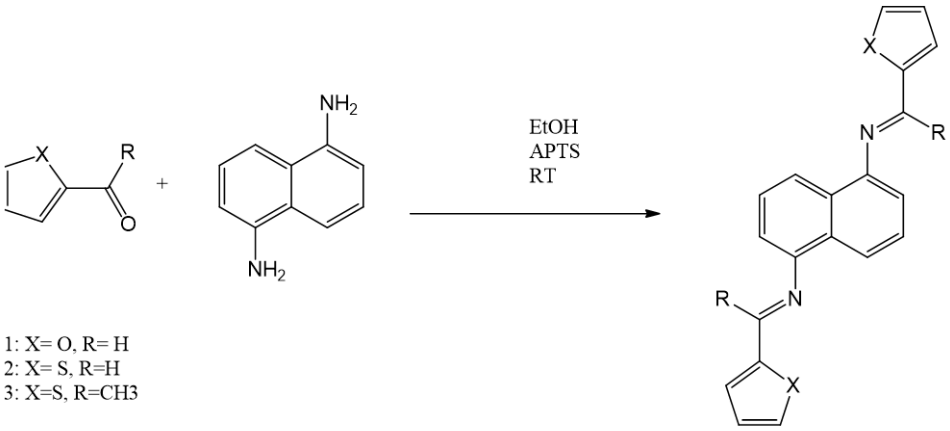
A series of α,α'-diimine ligands were prepared by condensation reactions of furfural, thiophenecarboxaldehyde or 2-acetylthiophene with primary diamines. The synthesis of ligands L1, L2 and L3 is carried out in a single step by condensation of two equivalents of aldehyde with a single equivalent of an aromatic diamine in ethanol at room temperature. These new compounds have been characterized by IR spectroscopy, NMR spectroscopy.



1: X= O, R= H
2: X= S, R=H
3: X=S, R=CH3

Key words: α,α'-diimine,NMR, IR spectroscopy.

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Comprehensive Analysis of Microstructure and Magnetic Properties in NdFe/MgO(001) Thin Films: Influence of Thickness and Heat Treatment

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Rare earth (R) and transition metal (T) based films hold significant potential for diverse magnetic applications, yet their structural and magnetic behavior remains intricately tied to growth and processing conditions [1]. This article presents a thorough investigation aimed at analyzing the microstructure and magnetic properties of NdFe/MgO(001) films. These films were fabricated through the evaporation of nanocrystalline Nd_3Fe_{29} powder, with varying thicknesses (t) and subjected to diverse heat treatments (T_a). The primary objective of this research is to provide a detailed understanding of how structural and magnetic behavior evolves based on these parameters, a level of insight not previously achieved. X-ray diffraction analysis was employed to determine the crystalline structure and track grain size evolution with film thickness. Scanning electron microscopy (SEM) and magnetic force microscopy (MFM) were utilized for direct visualization of magnetic domains and grain arrangement. Ferromagnetic resonance (FMR) measurements revealed variations in resonance fields and easy axes based on film thickness and heat treatments. The study explored correlations between magnetic properties such as saturation magnetization (Ms) and coercivity (Hc) with grain size, magnetic domain organization, and heat treatments. A noteworthy outcome was observed in a 250 nm thick NdFe/MgO(001) film annealed at 873 K, exhibiting outstanding properties including a coercivity of 5230 Oe, remanent magnetization of 211 emu/cm3, magnetic anisotropy field of 10,325 Oe, Ms of 396 emu/cm3, and a Curie temperature of approximately 388 K. Notably, this film featured an easy magnetization axis parallel to the film plane ($H_{FMR}(\parallel)$ = 9125 Oe > $H_{FMR}(\perp)$ = 5897 Oe). While providing valuable insights for magnetic material design and optimization, this study acknowledges limitations in exploring correlations between different properties. Future work will focus on simulations and theoretical modeling to address this research gap, contributing to a more comprehensive understanding of these characteristics.

Key words: Microstructure, Magnetic Properties, NdFe/MgO(001) Thin Films, Ferromagnetic resonance.

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Tunable Optical Properties In a 2D Organic-Inorganic Hybrid Material

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Low-dimensional organic-inorganic hybrid materials (OIHM) have garnered significant attention due to their versatile structural and photophysical characteristics. They hold promise for various optoelectronic applications, including the development of single-component white-light-emitting diodes. In this work, we introduce a novel two-dimensional (2D) lead-chloride compound. Within this compound, organic molecules envelop inorganic layers, formed by bridging between clusters without a specific orientation. When excited by UV-visible light, the hybrid material emits light across the visible spectrum, offering tunable luminescence based on the excitation wavelength. Remarkably, it even displays room-temperature phosphorescence visible to the naked eye. We delve into the origin of these optical properties by comparing the hybrid compound with its organic salt counterpart, revealing that clusteroluminescence is the underlying mechanism responsible for these unique optical behaviors.

Synthesis, crystal structure and DFT calculations of novel hybrid organic-inorganic compound, 3-methylbenzylammonium perchlorate

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The novel organic-inorganic hybrid compound of 3-methylbenzylammonium perchlorate has been successfully synthesized by slow evaporation technique at room temperature. This compound has been determined by X-ray diffraction analysis and characterized by FT-IR complemented with a quantum chemical study performed with DFT method. The 3D Hirshfeld surface and 2D fingerprint plots analyses have been used to examine the intermolecular interactions present in the crystal structure. The optical properties were investigated in the solid-state. The non-covalent interactions were studied on the basis of Reduced Density Gradient (RDG) and Atoms In Molecules (AIM). The HOMO-LUMO analysis is used to determine the charge transfer within the molecule. The molecular electrostatic potential (MEP) is used to determine the electrophilic and nucleophilic sites as well as the interactions of the hydrogen bond.

Keywords: DRX, DFT calculations, Hirshfeld surface, AIM, RDG, MEP.

Polyphenol content and antioxidant activities of solvent extracts from *Rhanterium sueaveolens*

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The plant Rhanterium sueaveolens has been traditionally employed in herbal therapy. Among the many bioactive substances found in it are polyphenols, which are naturally antioxidant. Rhanterium sueaveolens polyphenols have potent antioxidant effects that help save tissues and cells from oxidative damage. Our goal in this work was to extract the bioactive components from Tunisian Rhanterium sueaveolens utilizing a variety of extraction methods, including maceration, ultrasonication, and Soxhlet extraction. In this study, the potential of Rhanterium suaveolens as a source of stimulating bioactive components was evaluated by analyzing the phenolic content and antioxidant activities of extracts from the plant's flowers and stems. The appropriate analytical technique was applied to quantify the polyphenols. Additionally, the tests for DPPH and ABTS were used to determine the antioxidant activity.

The Rhanterium suaveolens extracts under investigation appeared to be very high in polyphenols, and all of them seemed to have good antioxidant and free radical scavenging properties, with the flower extracts being slightly more active than the rest.

The study's findings will shed important light on the plant's possible bioactive components as well as how well Rhanterium sueaveolens extracts when extracted using various methods. The plant's potential health benefits and use in the development of natural antioxidants will be better understood with the assessment of its polyphenol content and antioxidant activity.

Keywords: Rhanterium sueaveolens, extraction, polyphenols, antioxidant activities, DPPH, ABTS.

OPTIMIZATION OF AN ECO-FRIENDLY CEMENT MORTAR BY RESPONSE SURFACE METHODOLOGY

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The aim of this work is to valorize eggshell powder, glass waste and prickly pear cladodes juice from Opuntia ficus indica as partial cement replacement using response surface methodology particularly the Doehlert design. The main objective is to elaborate semi ecological cement with high mechanical strength and delayed setting time as well as to reduce the carbon dioxide emission and energy consumption from cement production. The obtained results revealed that a replacement of 8,45% of cement powder by the three types of used waste gave a cement with considerable mechanical strength of 31,5MPa and delayed setting time of 317 min compared to referred Cement (without replacement). Rheological behavior study of developed cement revealed that this one exhibited a pseudoplastic behavior with reduction in viscosity after incorporation of the three types of waste which is explained by the superplasticizing effect of polysaccharides contained in the cladodes juice.

Keywords: Portland Cement, semi ecological, Doehlert design, compressive strength, setting time, pseudoplastic behavior.

Modeling of essential oil extraction kinetics of Tunisian medicinal plants

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The present work deals with the modeling of essential oil extraction kinetics of three medicinal plants from southern of Tunisia (Salvia rosmarinus, Thymus and Juniperus phoenicea) using hydro distillation method. The extractions were carried out with a water/plant material ratio of 10 g/g, a heating power of 204 W and an extraction time up to 3 hours. The extraction kinetics determined for seven different plant samples (three individual plants and four mixtures) showed two diffusional extraction steps. Modelling was carried out using a non-stationary diffusion model and a first-order kinetic model. The results showed that the extraction process appeared to follow the non-stationary diffusion model for the majority of the samples studied.

Key words: essential oils, kinetic model, hydrodistillation, non-stationary diffusion, first-order kinetic.

Valorization of spent coffee grounds extract as a corrosion inhibitor of copper in NaCl solution

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The effects of spent coffee grounds (SCG) extract on the corrosion of copper in 3 wt % NaCl solution were examined. Extraction was performed using n-hexane as the extraction solvent for decoction. This extract was analyzed using Fourier-transform infrared spectroscopy (FTIR) and thermogravimetric analysis (TGA). An extract concentration of 0.2; 0.4 and 0.6 g/L were analyzed as inhibitors for copper corrosion in NaCl 3% solution, using electrochemical tests: potentiodynamic polarization and electrochemical impedance spectroscopy. The electrochemical measurements revealed that SCG extract acts as a cathode-type inhibitor for copper in saline media, mainly hindering the diffusion of oxygen molecules towards the substrate. In addition, the EIS results indicated that the organic compound was adsorbed onto the copper electrode.

Keywords: SCG, copper, FTIR, TGA, voltammetry around OCP, EIS.

Development of a Cyclodextrin-Based Bio-Adsorbent for the Removal of Pharmaceutical Contaminants

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Triclosan (TCS) and Paracetamol (PCM) are extensively used by humans: TCS as a widely distributed antibacterial agent in numerous personal care products, and PCM for its analgesic and antipyretic effects. However, due to their frequent use, these substances are commonly found in wastewater, persist through water treatment processes, and ultimately end up in surface water. These molecules can be ingested by humans and pose serious threats to human health. It is crucial to develop an economical and feasible procedure that ensures the simultaneous and effective elimination of TCS and PCM molecules [1]. To meet this criterion, the choice was made to use native cyclodextrins (α, β, and γ), employing citric acid as the grafting agent (for CD onto the cellulosic fibers) and for cross-linking (between CD molecules), in the presence of a specific catalyst for the esterification reaction in the acid/Cyclodextrin/Posidonia mixture. First, the native cyclodextrins are used to assess the complexation phenomenon with TCS and PCM in order to select the cyclodextrin that presents the most stable complex. The formation of an inclusion complex between a CD and these guest molecules has been examined using ^{1}H NMR. The stoichiometry and stability constant have been determined, demonstrating that β-CD is the cyclodextrin that forms the most suitable complexes. Second, The material resulting from the functionalization of these cellulosic fibers by β-CD was characterized using various analytical techniques such as Infrared Spectroscopy (IR), Zeta Potential, Light Microscopy, Thermogravimetry Analysis (TGA), and Scanning Electron Microscopy (SEM). These methods allowed for a qualitative characterization of the surfaces modified by CDs, as well as the determination of the grafting densities of β-CD achieved on the Posidonia surface.

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Metal-organic framework and conducting polymer based electrochemical sensor for high performance lead ions detection

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In this work, a conductive electrochemical sensor, HKUST-1@PANI, was successfully prepared by polymerizing the conductive polyaniline (PANI) polymer around the metal-organic framework HKUST-1. The resultant material was applied to construct a novel electrochemical sensor for the reliable detection of lead ions. Under optimized conditions, a linear detection of Pb^{2+} concentration range of 0.005 to 50 µM was repeatable with a 5 n M lowest level detection limit. Little to no interference effects from other co-existing ions allow the sensor to work in varing environments for practical application.

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Adsorption of porphyrin and phthalocyanine on graphene: Overview of theoretical investigation for heterojunction organic solar cell applications

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Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) approaches were employed to investigate the adsorption of phthalocyanines and porphyrins on graphene surfaces. Simplifying the structures of the studied pigments enabled the reproduction of experimental geometric parameters, facilitating the assessment of optical and electronic properties. Our findings reveal the superior performance of the ω-B97XD functional for such calculations [1]. A comparative analysis of theoretical vertical energies (Q_x and Q_y) and adiabatic energy ($E_{0\text{-}0}$) highlights the synergistic relationship between experimental and theoretical methodologies. Additionally, adsorption energies (E_{ads}) were quantified [2], demonstrating a consistent increase with graphene size [3]. The complexes based on cadmium and mercury exhibit promising values, facilitating their adsorption onto graphene substrates. This research contributes valuable insights into the interactions between organic pigments and graphene, with potential implications for advanced solar cell design.

Keywords: Porphyrins, Phthalocyanines, Graphene, BHJ organic solar cells, DFT, Electronic and optical properties

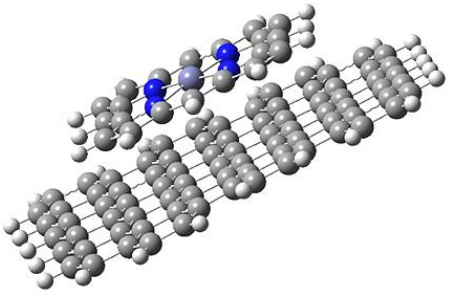

Figure : The 3D structure of the {ZnPr+graphene} system.

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DFT mechanistic study of the chemical fixation of CO by aziridine derivatives

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We report in this study, the reaction of CO with aziridine using density functional theory (DFT) taking into account the solvent and catalyst effects. In the case of methyl substituted aziridine, two pathways are proposed leading either to 3-substituted lactam or to 4-substituted lactam. The activation energy value of this reaction decreases as a functional of organic solvent. A comparative study of explicit and implicit solvatation models was conducted in order to provide a detailed solvent-reagent interaction investigation. Also, the corresponding reaction mechanisms and regioselectivity associated with aziridine conversions to β-lactams with carbon monoxide are found to be influence by solvent and catalyst. The present findings should allow better design of regioisomer β-lactams relevant for organic chemistry, medicinal, and pharmacological applications. [1-3]

Key words: β-lactam, CO cycloaddition, solvatation models, DFT.

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Neutron-Induced Nuclear Cross-Section Prediction for Germanium isotopes via Machine Learning Algorithms

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The neutron-induced reactions at low and medium energies have great importance in nuclear physics studies such as fusion and medical applications. One of the important parameters for nuclear reactions is the reaction cross-section. It can be obtained from experimental data or by different theoretical models. In this study, we apply machine learning (ML) algorithms to the regression analysis of the nuclear cross-section of neutron-induced nuclear reactions of Germanium isotopes. The data for the training of the machine was taken from the TENDL-2019 library for the cross-section data of potential nuclear reactions following the bombardment of various target materials by neutrons. Three ML models, Artificial Neural Networks (ANN), K-Nearest Neighbors (KNN) and, Support Vector Machines (SVM), were developed to fit nuclear data from the TENDL-2019 database in order to predict neutron induce reaction cross sections. The performance of each algorithm is determined and compared by evaluating the mean square error (MSE) and the correlation coefficient (R^2). The results show that cross-section data can be safely acquired using ML approaches, and the regression curve generated by our models is in good agreement with the nuclear data library that has been evaluated. From our study, ANN and KNN are found to be better compared to SVM algorithm. ML models can enhance classical physics-guided models and play a role in nuclear data analyses. They can be used as an alternative to the estimation of cross-sections for neutron energies of an unknown energy value.

Keywords: Neutron-induced reaction, cross-section, supervised machine learning, artificial neural networks, K-Nearest Neighbors, Support Vector Machines

CO_2 adsorption on modified graphene, DFT investigation

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The excessive concentration of CO_2 in the atmosphere has led to rising global temperatures, which, in turn, result in severe consequences like more frequent and intense heatwaves, melting ice caps, and extreme weather events. In order to combat CO_2 emissions and mitigate its impact on the environment, various strategies can be employed. However, the search for new materials for efficient capture and separation of CO_2 is highly desired in both environmental and industrial fields, generating significant interest. Our study has resulted in the proposal of the design of innovative materials for the capture and detection of CO_2, including the use of two-dimensional solid surfaces such as chlorine-decorated porous graphene, couronene, and hexagonal boron nitride. Hence, optimized geometries, adsorption energies, energy decomposition analysis, and Density of states (DOS) have been carried out using Density Functional Theory (DFT). These findings open up new prospects in the field of environmental chemistry and CO2 sequestration.

Keywords: DFT, energy decomposition analysis**,** halogen bond, σ hole, graphene

Investigations of sintered dry-pressed alumina using synthesized organic copolymer

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Polyelectrolytes containing both carboxylate and hydroxyl functions noted (PV2A) have been synthesized to provide the dual function of dispersant and binder for dry pressed alumina. The incorporation of PV2A in the ceramic formulation improved tensile strength of pressed products from low concentrations (1wt%), showing a good binding effect.

The effect of copolymer content and sintering temperature were examined on the microstructural and mechanical properties of sintered compacts. Characterized by a low glass transition temperature, PV2A copolymers have a plastic character. This quality ensured a high densification. Such property makes synthesized copolymers more promising than the industrial additives ensured a homogeneous microstructure of sintered parts and high relative density (99.2% with addition of 1wt% of PV2A against 97.7% in the presence of commercial PVA + PEG at 1650 °C).

The plastic character and the minimal amount of organic additives in the alumina formulation prevent microstructure defects during sintering, and improve the mechanical properties of sintered parts to reach a tensile strength of 357.5 MPa at T=1700°C with the addition of 2wt% of the copolymer.

Key Words: Organic Copolymer, sintered dry pressed alumina, glass transition temperature

Poly(ether-sulfone) modified silica gel for the adsorption of water pollutants

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Due to the development of human activities in the recent decades, notably in agricultural, industrial and civil sectors, water pollution was dramatically raised, causing serious environmental and health problems [1]. Among different contaminants, aromatic organic compounds attracted considerable attention due to their toxicity, non-biodegradability and carcinogenic nature [2]. Many scientists suggest hybrid organic-inorganic adsorbents, with high specific surface area and enhanced adsorption capacities [3]. In the present work, we describe the synthesis of a new organic-inorganic stationary phase from renewable resources. A silica gel coated with a semi-IPN network based on semi-biosourced poly(ether-sulfone) was studied for pollutant extraction. The developed adsorbent phase was tested for nine aromatic pollutants. An optimized composition of the semi-IPN network leads to a total adsorption of the selected pollutants.

Key words: Hybrid adsorbents, Semi-IPN Network, Poly(ether-sulfone), Adsorption.

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Investigation of physical properties of Al doped lead phosphate glasses

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Al doped lead phosphate glasses (AlLPG) as 40 % PbO, 40 % P_2O_5, (20-x) % Na_2O_3, x Al_2O_3, (x = 0, 1, 2, 3, 4 and 5 %) matrix system are prepared by the melt-quenching method. The physical properties have been performed using several techniques such as X-Ray Diffraction (XRD), Differential Scanning Calorimetry (DSC), Fourier Transform InfraRed spectroscopy (FTIR), Raman spectroscopy, UV-Visible properties and photoluminescence (PL). XRD confirms the amorphous character of the glasses. The optical spectra don't present significant effect and so no Al^{2+} absorption bands are detected. The Urbach energy ΔE_{urb} shows an increase with increase of aluminium amount which is related to the increase of the structural disorder degree as the rate of aluminium increases. Moreover, it's worthwhile to mention that it's for the first time that the PL of the Al doped lead phosphate glasses is investigated. Undoped glasses PL spectra reveal some impurities among them iron contamination. For doped glasses, the trace of iron impurities is still presented and the other impurities can be overlapped by the Al^{2+} ions transition. PL spectra exhibit as well emission bands corresponded to the Pb^{2+} single and complex centers.

Fe-MOF: A High-Performance Electrochemical Sensor for Simultaneous Detection of Hydroquinone, Catechol, and Resorcinol

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MOFs are particularly notable for their exceptionally large surface areas, adjustable pore sizes, and versatile internal surface properties. These characteristics make them highly promising for a range of applications[1]. This research highlights the effective synthesis of Fe-MOF (known as Mill 101) and its utilization as an electrochemical sensor for the precise detection of environmentally concerning dihydroxybenzene isomers. The Fe-MOF was successfully deposit on SPCE without using any binders and its electrochemical behaviour was investigated. The proposed sensor displays excellent electrocatalytic activity toward the oxidation of HQ, CC and RS. Under the optimized conditions, the electrochemical sensor shows a wide linear response in the concentration range of 1–700 µM, 1–700 µM and 1–290 µM with a detection limit of 0.2 µM, 1 µM and 0.1 µM for HQ, CC and RS, respectively. In addition, the sensor has superior sensitivity and good reproducibility. The fabricated sensor was also applied for the determination of DBIs in the real water samples with satisfying results.

Keywords: Electrochemical sensor, Metal-organic frameworks, Dihydroxybenzene isomers

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THE STUDY OF THE USE OF NANOFLUIDS TO IMPROVE THE PERFORMANCE OF ABSORBERS FOR REFRIGERATING MACHINES

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Among the various refrigeration systems, vapor compression and vapor absorption systems are the most used systems. The compressor, condenser, expander and evaporator constitute the four main components of a vapor compression system. In a vapor absorption refrigeration system, an absorber-generator-pump assembly replaces the compressor of the vapor compression system. Examples of this heat source include steam sources, hot exhaust gases and solar energy. This study focuses on the absorption system. Two commonly used absorption systems are the lithium bromide/water ($LiBr/H_2O$) refrigeration system and the ammonia/water (NH_3/H_2O). The latter system in which water (H_2O) is the absorbent and ammonia (NH_3) is the refrigerant is capable of reaching refrigeration temperatures lower than ancient system in which water is the coolant. The absorber constitutes a key device in absorption refrigeration machines and represents a significant part of the overall price of the system. The function of an absorber is to improve the concentration of the lean refrigerant solution by absorbing the refrigerant vapor. Poor absorption of the refrigerant in the absorber can significantly reduce the performance of the entire device. In order to increase the performance of these systems, one of the solutions consists of using nanofluid, which is likely to improve the heat, and mass transfer processes of the refrigeration system by absorption. Recently, nanofluids have been an active area of research due to their greatly improved thermal properties. In this context, this study aims the improvement of the absorption of refrigerant by a poor solution, by considering the two configurations of the most used absorbers, which are falling film and bubble absorbers.

Calculations codes were developed using MATLAB and COMSOL MULTIPHYSICS softwares to carry out the simulation of the analyzed phenomena. The results obtained show that the transfer of matter and heat in the presence of nanoparticles is greater than that of the base fluid and that the efficiency of the nanofluid becomes greater than that of the fluid basis for a low Reynolds number and a higher inlet temperature of the lean solution.

Thermal energy storage Processes : Recent applications and innovations

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Thermal energy storage is a crucial component in the efficient utilization of renewable and waste heat energy sources. This paper presents a systematic literature review of various thermal energy storage processes, including sensible, latent, and thermochemical storage methods. The review encompasses the current state of the art, challenges, and opportunities in the field. Furthermore, it explores recent innovations and emerging technologies that have the potential to enhance the efficiency and applicability of TES systems. Key topics covered include materials advancements, integration with renewable energy sources, and novel storage system designs. By providing a comprehensive analysis of the existing knowledge base and highlighting recent developments.

Key words : thermal energy storage, processes, innovations

Optimizing Heat Storage in Integrated Solar Water Heaters: Comparing Storage Materials for Improved Efficiency

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Solar Energy, although renewable, still faces a heat storage challenge, especially in integrated solar water heaters. These systems experience significant nighttime cooling. The choice of storage material can influence the lifespan of storage tanks, the amount of stored heat, and its release rate. In this study, we compare five heat storage materials: sand, concrete, clay, Phase Change Materials (PCMs), and water as a reference element for comparisons. The PCM used here is commercial paraffin, although other materials offer higher fusion enthalpy. During daytime heating, the PCM may not reach the highest temperatures because the received solar energy is used for its phase change. However, in terms of stored heat quantity, the PCM excels due to its high latent heat. Additionally, for nighttime cooling, the PCM maintains a high temperature.

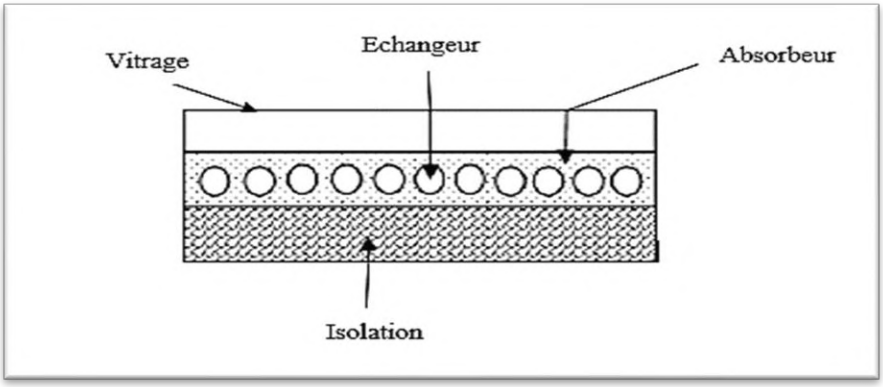

Figure 1. *Diagram of an integrated solar water heater with storage*

Keywords: Hot Water, Solar Energy, Integrated Storage Collector, Storage Materials, Concrete, Sand, Clay, Paraffin

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Laser-Induced Graphene Interdigitated Electrodes Modified with Redox-Active Polymers for Energy Storage

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Nanomaterials play a pivotal role in advancing new tools for biomedical analysis, environmental monitoring, and energy storage (1). Use of carbonaceous materials to fabricate electrodes is a highly sought-after approach, given their high potential for charge storage (2). Laser-induced graphene (LIG) technique has been identified as a promising, cost-effective, and high-throughput method for producing carbon-based electrodes (3). Polyimide-based LIGs have the potential to function as good electrode materials for supercapacitors (4).
Our research focuses on enhancing the capacitive performance of PI-based LIG interdigitated electrodes for energy storage in supercapacitors. Post functionalization with conductive polymers can significantly enhance the specific capacitance of a system by maximizing the electrical capacitance of the double layer and adding a pseudo-capacitive component, thus improving its overall energy storage performance. The present supercapacitor, elaborated by modifying the surface of a PI-based interdigitated LIG with electrochemically deposited poly(methylene blue), exhibits a remarkably wide and stable potential window up to 3.0 V thanks to the use of a PVA/$HClO_4$ gel electrolyte, providing an improved surface capacitance, energy density and power density. Indeed, the specific capacitance increased by 253% after modification of LIG. Notably, this supercapacitor also demonstrates exceptional cycle stability over 5,000 cycles. These results highlight the potential of this supercapacitor for energy storage capability.

Key words: Laser-induced graphene, Energy storage, Redox polymer, Supercapacitor.

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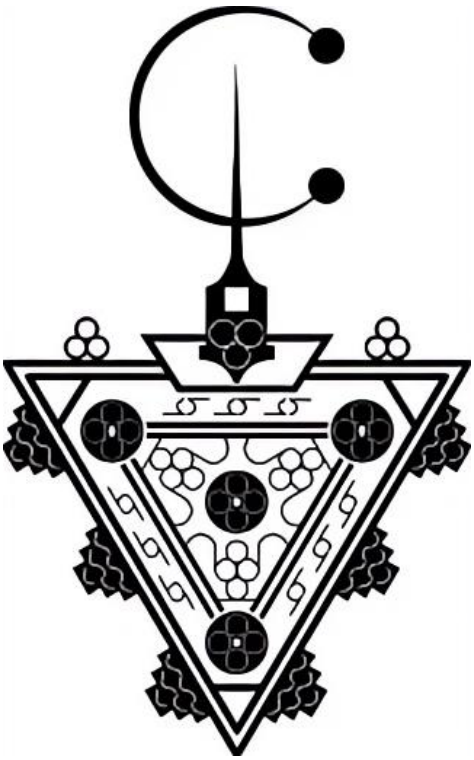

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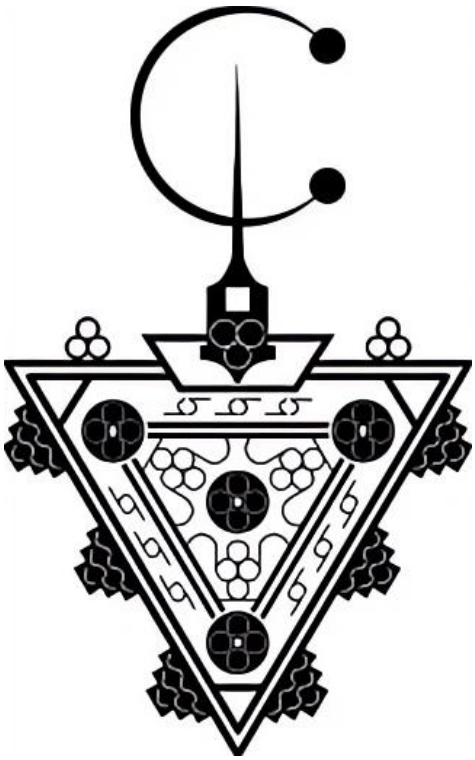

Abstracts of Poster Communications

Synthesis, characterization and chromium ions adsorption of calix[6]arene-tetraester-silylated clay nanocomposite

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In this investigation, calix[6]arene-tetraester-silylated-clay (SC-C[6]) is prepared, and characterized. The adsorption of chromium ions onto SC-C[6] as a function of pH solution, contact time, initial Cr(VI) concentration and effect of temperature is studied through batch experiments. The removal towards Cr(VI) increased with decreasing of pH solution : from 7.5 to 1.5, while it decreased with increasing of initial Cr(VI) concentration and temperature. The maximum Cr(VI) adsorption capacity for SC-C[6] reached at pH 1.5, 10.4mgL^{-1}, 25°C and 1h, and the mechanisms may include electrostatic interaction and chemical interaction between the nanocomposite and Cr(VI) ions.

Inclusion complexes study of a series of molecules with differents Cyclodextrins

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Introduction: Cyclodextrins (CDs) are a group of cyclic oligosaccharides produced from starch or starch derivatives. They contain six (αCD), seven (βCD), eight (γCD), or more glucopyranose monomers linked via α-1,4-glycosidic bonds. CDs have a truncated cone shape with a hydrophilic outer wall and a less hydrophilic inner wall, the latter forming a more apolar internal cavity. Because of this special architecture, CDs are soluble in water and can simultaneously host lipophilic guest molecules. The major advantage of inclusion into CDs is increased aqueous solubility of such lipophilic substances. Accordingly, we present studies where the complexation of natural compounds

Material and Methods: In present work the complexation of series of molecules with two kinds of cyclodextrins (CDs), native β-cyclodextrin (β-CD) and α-cyclodextrin (αCD), have been investigated by UV and 1H-NMR spectroscopy. The stoichiometric ratios, inclusion constants have been determined by Job and Bensi Hildbarnd methods.

Results: The different complex shows a higher antioxidant efficacy both in terms of capacity and rate of scavenging DPPH radical. The antioxidant activity of in free form has little difference with the differents guest in complexed form at the same concentration, this result indicates that the complexes formed maintained the Res antioxidant activity. This work shows the potential usage of Res/CD complexes.

Conclusion: Based on this study, we concluded that formulation of resveratrol and the other molecules with different cyclodextrin can improove the stability of resveratrol and incres the antioxidant activity.

Keywords: *Resveratrol*, Polyphenols, antioxidant activity, Cyclodextrin.

Synthesis of iron copper phosphate catalyst for CC coupling reaction

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Almost all organic compounds that contain heterocyclic nitrogen are biologically very active and have been introduced into the synthesis of pharmaceutical molecules. This is what motivated us to make the synthesis of propargylamine using the c-c coupling pathway.

To ensure the best yield for this reaction and for the fastest collection of propargylamine we used metal catalysts of binary copper iron phosphate type to activate the reaction of the side and also because of the rare studies that make this.

Keywords: Catalyst, nanoparticle, syntheses

A New Nanocomposite Based on Poly (O-Toluidine)/Graphene Oxide and a Natural Polymer for Treatment and Removal of dye Pollutants from the Aquatic Environment

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The idea of this project is to prepare a new nanocomposite based on poly (o-toluidine)/graphene oxide and a natural polymer such as cellulose (NCs) and use it to treat and remove a dye pollutant as Acid Red 1 from the aquatic environment. All the physical properties of the new polymers such as FTIR, XRD, TEM, SEM, BET will be studied. In order to study the removal effectiveness of the NCs with various parameters, including adsorbent dose, pH and temperature of the solution, shaking time, and ionic strength. The experimental data of the adsorption process showed that NCs can remove most of the A.R dye within 75 minutes, at pH 2.0 with an adsorption efficiency of 99.4% using 25 mg of solid phase NCs, and with adsorption capacity 31.1 mg/g of A.R dye on NCs. The removal process of A.R dye on NCs solid phase was studied kinetically using different kinetic models, and the results data confirm that the pseudo second-order kinetic model was able to describe the adsorption process. The removal process was studied thermodynamically, and the results data confirm that the removal was spontaneous, endothermic in nature, and associated with increase in randomness. Finally, the efficiency of NCs was studied by removing A.R dye from three different real samples, and the results data confirms that NCs has great efficiency in removing A.R dye from aqueous solution for four consecutive cycles.

New copper(II) complexes supported by azomethine ligands: Synthesis and characterization

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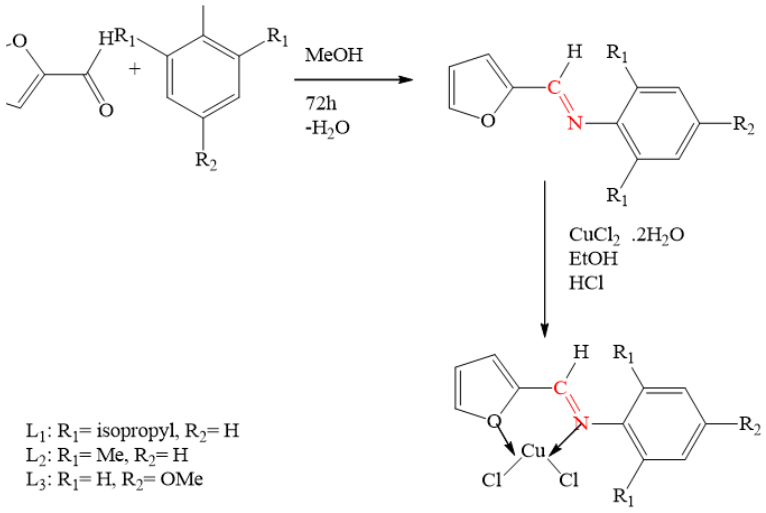
A series of azomethine ligands were prepared by condensation reactions of furfural with anilines [1,2]. Ligands, 2-(N-2,6-diisopropylphenylformimino)furan (L1) and 2-(N-4-methoxy-phenylformimino)furan (L2) were obtained by condensation reactions of the respective anilines with furfural. The reaction of copper (II) chloride dihydrate with one equivalent of the ligands L1 et L2 in ethanol at room temperature, always afforded the corresponding complexes $LCuCl_2$ (L= L1 or L2) with high yields. These new complexes have been characterized by IR spectroscopy, NMR spectroscopy, UV-VIS.



Key words: Bis(diimine), Copper (II) chloride dihydrate, IR spectroscopy.

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Solid-Phase Extraction using Functionalized Magnetic Biochar Composite for the Determination of Acid Caffeic in water Samples

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This study aims to concurrently achieve qualitative and quantitative determination of hydroxycinnamic acid (specifically caffeic acid) in biological samples. Magnetic solid-phase extraction (MSPE) is employed for sample treatment and preconcentration before analyte separation, gaining increasing attention due to its numerous advantagesHaut du formulaire. The use of magnetic nano sorbents modified with inorganic and organic species has become widespread in studies on solid phase extraction (SPE) due to its numerous unique properties. The synthetized nanocomposite was characterized by, scanning electron microscopy, Fourier transform infrared spectrophotometry, and X-ray diffraction. Various experimental parameters were optimized such as contact time, pH, sample volume, eluent volume and adsorbent mass. The results demonstrate the potential use of functionalized biochar as new adsorbent in solid-phase extraction devices for the extraction of caffeic acid from biological.

Keywords: biochar, hydroxycinnamic acid, nano-composite, magnetic solid phase extraction, biological samples.

Synthesis and characterization of pyrazolate metal organic framework thin film

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Metal Organic Frameworks (MOFs) are a promising class of porous nanostructured materials constructed from metal ions and organic linkers [1]. Moreover, the Surface-Mounted Metal Organic Frameworks (SURMOFs) represent a challenge facing the development of future technological breakthroughs. The processability of MOFs as films on surface together with their major features is broadening their range of applications to areas such as gas adsorption and separation, photovoltaics, and sensor development [2]. In this work, we have studied the effect experimental conditions, including the metal/ linker molar, on morphology of Zn-NDIP thin film prepared from Zinc (II) hydroxide nanoparticles via layer-by-layer growth method. The structural and morphological studies of obtained film were characterized using ATR-FTIR, X-ray diffraction (XRD), UV/VIS spectroscopy and optical microscopy. We found that the Zn /NDIP molar ratio used in the secondry growth step could control particle sizes and shapes of the resulting Zn-NDIP materials.

Key words : SURMOFs, Zn-NDIP, Zinc hydroxide

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Natural Apatite-Metakaolin Supported TiO_2 Mesoporous Membrane with low cost for environmental applications

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This study suggested the manufacture of a TiO_2-tight ultrafiltration membrane supported on an inexpensive ceramic substrate made of metakaolin and natural apatite. Three samples were made by combining metakaolin and natural apatite in weight ratios of 25:75 (MK25), 50:50 (MK50), and 75:25 (MK75) in order to improve the substrate composition. The samples were then sintered for two hours at 850, 900, 950, and 1000°C. Microstructure, porosity, and mechanical strength of the produced samples were examined in relation to the impact of sintering temperature and metakaolin content. The results showed that both the temperature and metakaolin content increased, the porosity dropped. In contrast, the mechanical strength increased. The ideal parameters were found to be MK50 composition and 950°C. The resultant substrate had a 4.4 MPa compressive strength, 33% porosity, and an average pore size of 2.2 μm. The deposition of the TiO_2 top layer was preferred over the alumina intermediate layer in order to construct an ultrafiltration membrane devoid of cracks. The resulting membrane has a water permeability of 5.6 $L.h.^{-1}m.^{-2}bar^{-1}$ and a pore size of 6.8 nm. The ability of the membrane to remove both anionic and cationic dyes was examined. Anionic and cationic dyes have a high clearance rate, according to UF tests. In particular, it was discovered that these dyes may be removed at rates higher than 75% without changing the solution's pH.

Keywords: Natural apatite, metakaolin, Al_2O_3, TiO_2, UF membrane, dye

Synthesis, crystal structures, spectroscopic characterization, and evaluation of antitumor activities of two new decavanadate compounds against U87 human brain cancer cells

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Glioblastoma (GBM) is the most fast-growing and aggressive brain tumor [1]. Unfortunately, GBM cells demonstrate inherent resistance to conventional therapeutic approaches. In this context, new potential drugs based on decavanadates are being developed as possible treatments for brain tumors [2]. Two novel decavanadate compounds: tetra-[methylimidazolium] dihydrogen decavanadate(V) $(C_4H_7N_2)_4[H_2V_{10}O_{28}]$ and hexa-[methylimidazolium] dihydrogen decavanadate(V) dihydrate $(C_4H_7N_2)_6V_{10}O_{28}{\cdot}2H_2O$, are characterized by single-crystal X-ray diffraction, by FT-IR, UV-Vis and ^{51}V NMR spectroscopies. The compounds crystallize in the monoclinic system space group $P2_1/c$ *and* $P2_1/n$ respectively. Important intermolecular interactions in both structures are N-H···O and O-H···O hydrogen bonds and π-π stacking interactions between the organic cations. The Hirshfeld surface (HS) and their relative two-dimensional fingerprint plots (2D-FP) reveal that the two structures are dominated by O…H/H…O and H…H contacts. Interestingly, these decavanadate salts $(C_4H_7N_2)_4[H_2V_{10}O_{28}]$ and $(C_4H_7N_2)_6V_{10}O_{28}{\cdot}2H_2O$ inhibit the viability of U87 cells with IC_{50} values of 0.22 µM and 0.96 µM, respectively, after 72 h of treatment.

Keywords: Decavanadate, Glioblastoma, U87, Anticancer activity

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$Fe_3O_4@Ti_3C_2$ MXene hybrid as a novel adsorbent material for environmental remediation

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Most consumer items, including textiles, paper, leather, food, and cosmetics, are colored using synthetic dyes that, when combined with other auxiliary chemicals, form large discharges that threaten aquatic life and humans with poisonous, carcinogenic, and mutagenic effects. The removal of dyes can be accomplished utilizing a variety of treatment methods, including as ion exchange, precipitation, coagulation-flocculation, filtration, liquid-liquid extraction, electrochemical methods, and adsorption. Adsorption is considered one of the most efficient removal techniques. Nothing excites the community of material scientists more than the idea of a new family of two-dimensional (2D) materials, especially one with a large range of potential compositions and tailorable features for varied uses. The most recent instance of the 2D materials is the MXene family. MXene exhibits good chemical stability, tunable chemistry and high hydrophilicity, and has a strong negative surface charge. Many surface functionalization techniques have been cleverly developed recently to increase the potential of MXenes in various sectors, including surface-initiated polymerization and single heteroatom doping.

This study investigated the possibility of preparing, and characterization of $Fe_3O_4@Ti_3C_2$ NPs as a novel nanomaterial and their application for the removal of malachite green dye (MG); as an example of organic dyes, from water. The prepared $Fe_3O_4@Ti_3C_2$ NPs were characterized by various techniques, and the results demonstrated the homogenous distribution of the prepared NPs. The effect of different operational parameters affecting the removal process were explored, and the dosage of $Fe_3O_4@Ti_3C_2$ NPs, the initial concentration of MG, the pH and temperature of the solution, and the exposure period were all studied and optimized. Most of the MG dye were remove within 60 minutes, with removal capacity of 3.14 mg/g. The removal was studied kinetically and thermodynamically, and the results showed the applicability of the pseudo-second order kinetics; compared with other kinetic models, and the spontaneity of the removal process. The $Fe_3O_4@Ti_3C_2$ NPs were used for the removal of MG dye from real environmental water samples and the results revealed the successful remediation of the real samples from the organic dye by the $Fe_3O_4@Ti_3C_2$ NPs. Accordingly, $Fe_3O_4@Ti_3C_2$ NPs could be considered as a potential adsorbent for the environmental remediation of polluted water.

Keywords: Mxene; $Fe_3O_4@Ti_3C_2$ NPs; removal; Malachite green dye; remediation

Removal of Malachite green dye utilizing graphene oxide/nanoclay nanocomposite: Kinetics thermodynamic studies and environmental application

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Herein, graphene oxide/nanoclay nanocomposite was prepared, characterized and used for the removal of malachite green dye from environmental water samples. The effects of different operational paramters on the removal proc ess was studied; graphene oxide/nanoclay nanocomposite mass, removal time, solution pH, ionic strength, and temperature had been explored. The optimum removal capacity of malachite green dye by the graphene oxide/nanoclay nanocomposite obtained was about 14.48 mg/g using 0.025 L of Malachite green dye solution with 5 mg/L concentration, and graphene oxide/nanoclay nanocomposite 7.5 mg within 120 minutes, at pH 4, and 298 K. The removal process was studied kinetically as well as thermodynamically, and the findings showed the pseudo-second-order kinetic model suitability, electrostatic, endothermic, chemical, and spontaneity nature of the removal process. Moreover, graphene oxide/nanoclay nanocomposite could be used for three consecutive times for the efficient removal of Malachite green with high efficiency. Finally, the graphene oxide/nanoclay nanocomposite applicability for removal of Malachite green in different spiked Red Sea water, waste water, and tap water sample was investigated and the graphene oxide/nanoclay nanocomposite showed a great potential application to removing Malachite green from the environment.

Keywords: graphene oxide; nanoclay; water treatment; malachite green; Kinetics; Thermodynamics

DEVELOPMENT AND CHARACTERIZATION OF POLY (VINYLIDENE FLUORIDE-CO-HEXAFLUOROPROPYLENE) (PVDF-HFP) NANOFIBER NANOCOMPOSITE MEMBRANES BY ELECTROSPINNING PROCESS FOR MEMBRANE DISTILLATION APPLICATIONS

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Protecting freshwater supplies and preventing contamination of groundwater, surface water, and ocean have become major challenges worldwide. Because our planet's freshwater supplies are limited, saltwater desalination and water treatment are the only viable methods for addressing the water problem. Membrane distillation has made remarkable progress in terms of nanofiber manufacturing and practical applications in recent years. Membrane wetting resistance is the main obstacle to membrane distillation (MD). The creation of membranes with the highest level of hydrophobicity was suggested as a remedy for this problem. In order to purify water, hydrophobic electrospun Poly (vinylidene fluoride-co-hexafluoropropylene, PVDF-HFP) nanofiber membranes were created and utilized in the direct contact membrane distillation (DCMD) method. Weights of nanocomposites were added in order to study their effect on improving the structural structure and mechanical and physical properties of the membranes. The PVDF-HFP polymer was dissolved in a mixture of N,N-dimethylformamide (DMF), acetone and successive quantities of graphene oxide (GO) and carbon nanotube (CNT) nanoparticles, were used to make the Electrospun Nanofiber Membranes. Constant working conditions are used, including voltage, needle and plate distance, flow rate, and so on. It was noted that increasing the heat post-treatment to 130 °C resulted in the formation of crosslinked ENMs, which improved their mechanical and physical properties. This was demonstrated by examining the thermal properties, crystal structure and phases by differential scanning calorimetry (DSC) and FTIR spectroscopy. Scanning Electron Microscopy (SEM) and Atomic Force Microscope (AFM) results showed that grafting PVDF-HFP with varied concentrations of nanoparticles and heat post-treatment improved the morphological structure of ENMs. The ENMs developed had excellent porosity of greater than 60%, uniform pore size and high hydrophobic qualities in general, where the contact angle was between 110° - 131°. Nanocomposites leads to an increase in elastic modulus and tensile strength All membranes had a high pure water flow value of about 30.00 - 48.00 L $m^{-2} \cdot h^{-1}$. Salt rejection was also found to be 99%. ENMs containing nanoparticles can provide an innovative and easy way to obtain more efficient, high-performance membranes in water desalination and water treatment.

Key words: Membrane distillation, Electrospinning Nanofibers Membrane, Poly(Vinylidene fluoride-co-Hexafluoropropylene, PVDF-HFP), Hydrophobic membrane, Nanocomposites.

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Optoelectronic characterization of quaternary alloy

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Ceramic-based quaternary II−VI materials have attracted much interests because their constituent elements have important characteristics, high characteristics of structure and optic applicable for digital recording heads, telecommunications, transformers, computers, sensors, photovoltaics, antibacterial and others. The $MgZnFe_2O_3$, $CoZnFe_2O_3$ and $NiZnFe_2O_3$ quaternary alloys nanoparticles are tetrahedral materials of chalcopyrite structure. They have been prepared by green technique; their structural properties are varied as atomic number varies. Due to limited or unavailability resources of the mentioned quaternary alloys nanoparticles, the cost is a challenge. However, green synthesis has reduced their cost.

Nanotechnology and Dry Powder Inhaled efficiency

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LNCM Tunisia

Dry powder inhaled (DPIs) medicines can be considered as an effective method for treating not only usual respiratory diseases but also other serious diseases as lung cancer and tuberculosis.

Improving the bioavailability and stability of DPIs is always the major challenge for pharmaceutical industries. To deal with: scientists developped nano-particules in order to master particles size and nature.

In this communication we will demonstrate three relevant subjects:

First: the impact on stability and bioavailabiliy of DPIs when developing nanoparticules.

Second: the enhancement of the DPIs quality, efficacy and safety when practicing nanotechnology.

Third: the major progress seen in complicated pulmonary diseases therapies when including nanoparticules in the DPIs formulations.

Key words: Dry powder inhaled, bioavailability, nano-particules, pulmonary diseases therapies

Synthesis, Physicochemical characterization, Crystal structure and Hirshfeld surface Analysis of a dinuclear Nickel complex $[Ni(H_2PO_4)_4(C_{12}H_8N_4)_2]$ and study of its antimicrobial and anti-virulence potential

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A dinuclear Nickel(II) complex was successfully synthesized and characterized by FT-IR, UV spectroscopy and single-crystal X-ray diffraction (XRD). The crystal structure of the compound revealed a triclinic system with space group *P*-1. The complex is composed of two Nickel atoms, two 1,10-Phenanthroline ligands, and four phosphate groups, with two of the phosphate groups forming bridged dinuclear units.

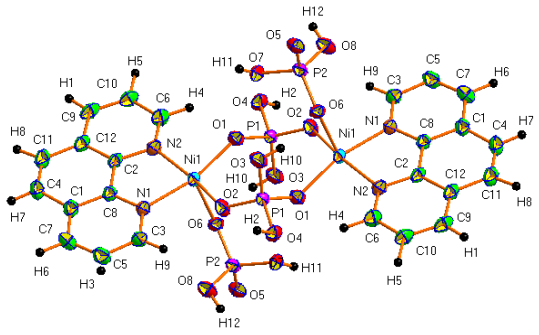

Fig.1 Perspective view of the complex Di-μ-hydrogen phosphato-κ^2 O,O'-bis[(hydrogen phosphato)(1,10-phenanthroline-κ^2 N,N')nickel(II)]

Within this crystalline phase, the crystallographically independent cations were examined in terms of their corresponding Hirshfeld surface. The formation of a three-dimensional network structure is stabilized by O-H...O hydrogen bonds between the bridging coligands.

The new complex highly inhibited the microbial growth, it interrupted the biofilm formation. The strong anti-virulence effect encourages its future application in the formulation of new therapeutic agents.

Key words: XRD, Dinuclear, Hirshfeld Surface analysis, antimicrobial, anti-virulence.

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The potentiel of lignocellulosic biomass for magnetic solid phase extraction of naproxen from saliva samples

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Plant waste materials, including almond, peanut, and walnut shells, serve as abundant biomass sources for biochar production via pyrolysis. This study presents the synthesis and characterization of three biochars derived from these materials, followed by their magnetization to enhance adsorption properties. Magnetized biochars were assessed for their efficiency in extracting naproxen, a common nonsteroidal anti-inflammatory drug, from saliva samples using LC-MS. Results highlight the potential of these biochars as effective adsorbents for naproxen extraction from complex biological matrices. This research promotes the utilization of plant waste materials and underscores the promising applications of magnetized biochars in pharmaceutical analysis, particularly in drug monitoring and pharmacokinetics. These findings have significant implications for environmentally friendly and cost-effective drug extraction and analysis

Key words: Magnetic Phase Extraction (MSPE), Lignocellulosic biomass, Saliva, Naproxen, LC-MS.

Antibiotic Removal using Amorphous Perlite: Batch/Photo-Adsorption

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This study delves into the utilization of natural perlite mineral for the oxytetracycline (OTC) removal from aqueous solutions. The investigation centers around crucial variables including contact time, initial OTC concentration, and temperature. The optimal conditions were pinpointed as a contact time of 113 minutes, an initial concentration of 178 mg/L, and a temperature of 318 K. The kinetic analysis revealed that the experimental data exhibited a closer alignment with the pseudo-first order model (R^2 = 0.9698). To comprehend the adsorption behavior, the Freundlich model showcased a favorable fit, indicating that OTC adsorption transpired across multiple layers on the heterogeneous surface of the raw Perlite. Furthermore, a thermodynamic inquiry unveiled the spontaneity, physisorption, and endothermic nature of the adsorption process. Lastly, the perlite's photocatalytic prowess was assessed, underscoring an augmented removal efficiency of OTC from 81.11% to an impressive 99.97% when subjected to solar radiation.

Graphical Abstract

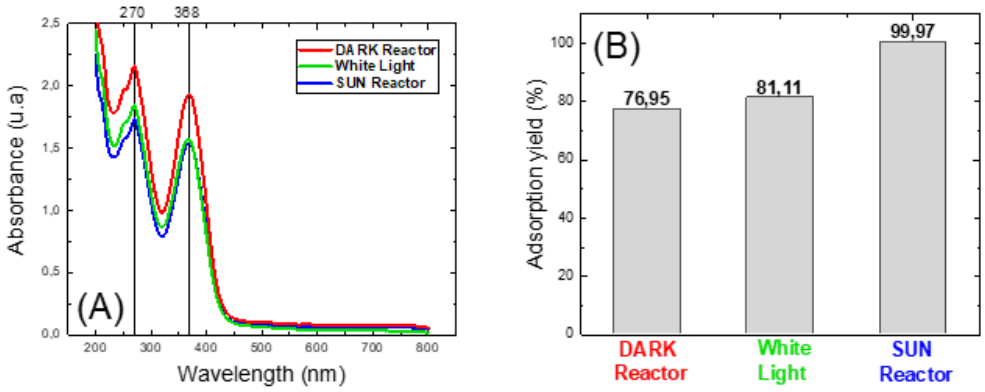

Figure: UV Spectra and yield's histograms of OTC adsorption onto Perlite into Dark, White light and under sunlight

Experimental study of the section X($NaNO_3$)/X($TlNO_3$) = 1/9 in the $LiNO_3$+$NaNO_3$+$TlNO_3$ ternary system

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Phase equilibrium diagrams are a very important tool in the field of materials science for alloy design and material synthesis. Indeed, phase diagrams are necessary to predict the thermal behaviour and the microstructure evolution of mixtures with temperature. However, the experimental determination of phase diagrams of the ternary systems over a wide range of compositions and temperatures is time consuming and costly. For these reasons, Calphad (Calculation of Phase Diagram) approach is the preferred method. The essence of Calphad method is to obtain a set of self-consistent thermodynamic parameters gathered in a database. This database including thermodynamic description of unary and binary phases can be used to calculate ternary phase diagrams in many instances. Experimental work is then required for confirmatory purposes and not for the determination of the whole diagrams [1].

In order to check the correctness of the predicted phase diagram of the $LiNO_3$+$NaNO_3$+$TlNO_3$ ternary system obtained in our previous work [2], the vertical section X(NaNO3)/X(TlNO3) = 1/9 was studied experimentally using the technique of simultaneous simple and differential thermal analysis. A satisfactorily agreement between the calculation and the experimental data was obtained.

Key words: Phase diagram, Calphad, LiNO3+NaNO3+TlNO3, vertical section.

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Stabilization of Tetrachloride with Mn (II) Complex and 4-Tert-Butylpyridinium Organic Cation: Elaboration of the Structure and Hirshfeld Surface, Optical, Spectroscopic and Thermal Analyses

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$[C_9H_{14}N]_2[MnCl_4]$ (**I**) and $[C_9H_{14}N]_2[CoCl_4]$ (**II**) are isostructural compounds produced via gradual evaporation at room temperature. Both compounds consolidate in the tetragonal space group $I\bar{4}2d$ (No. 122), as shown by single-crystal X-ray diffraction observations. A slightly deformed tetrahedral geometry is formed by four chloride atoms around each cation M^{II} (M = Mn or Co). The $[C_9H_{14}N]^+$ groups and the isolated $[MCl_4]^{2-}$ units are connected via C–H…Cl and N–H…Cl H-bonds to form sheets parallel to the $(10\bar{1})$, $(0\bar{1}1)$, (011) and (101) planes. The morphology and the chemical composition of compounds (**I**) and (**II**) were determined here using SEM and EDX. The functional groups contained in both compounds were determined using FT-IR spectroscopy. The study of the optical characteristics showed that the two compounds exhibited semiconductor behavior. The thermal analysis (TGA-DTA) was used to determine their thermal stability.

Key words: X-ray diffraction, SEM/EDX, optical absorption, vibrational study, thermal analysis.

Unraveling Electronic and Transport Properties of Carboxylic Acid-Modified Graphene Monolayers for Highly Selective Ammonia Sensing

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Graphene bearing organic functional groups chemically tethered to its surface via covalent bonds can find several applications in the sensing of gas, heavy metal ions, and other target species of interest. Herein, we used DFT simulations to study the thermodynamics of graphene functionalization with substituted carbenes [1], and the use of the resulting adducts to detect gaseous nitrogenated compounds-focusing on ammonia, methylamine, dimethylamine, and trimethylamine. We find that the modified materials can interact with the amines, selectively also in the presence of other gases such as CO_2, SO_2, H_2S, and CH_4. Changes in the electronic properties of the system upon adsorption such as charge density, Löwdin partial charges, and projected density of states were used to analyze the interaction. Furthermore, by modeling the conductance of the functionalized graphene bare and in the presence of ammonia, we show that quantum conductance and the integrated currents are sensitive to functionalization and, importantly, to the presence of ammonia under determined conditions, which in principle allows tuning the sensitivity of the resulting device [2]. Our work thus clarifies the principles governing this phenomenon. Carbene-functionalized graphene is concluded to be a potentially good candidate to replace noble-metal-modified graphene for the detection of ammonia/amines in chemoresistance or field-effect transistor-based sensors [3].

Keywords: Graphene; Gases; Sensors; DFT; Cycloaddition.

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Crystal structure and bioassay of a novel pyrazolone tested as an acetylcholinesterase inhibitor

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Pyrazolone derivatives have recently whetted much interest among researchers due to their versatile applications in various fields. In this work, we describe the condensation of thiosemicarbazide and tosylhydrazine with ethyl acetoacetate utilizing triethylamine as a basic catalyst.

The obtained compound $C_{11}H_{12}N_2OS$ crystallizes in the monoclinic symmetry, space group $P2_1/c$, with the following parameters a = 12.821 (9) Å, b = 7.588 (3) Å, c = 11.354 (5) Å, β = 94.828 (2) °, Z = 4 and V = 1097.400 (8) $Å^3$.

Inhibiting AChE activity is one of the main therapeutic interventions in the treatment of Alzheimer's disease (AD), hence docking studies were conducted for the reference substance rivastigmine and the produced pyrazolone against human acetylcholinesterase (AChE). Based on the binding position, rivastigmine was occupied in the central active site cavity of AChE whereas the created compound was at the site located in the deep cavity of AChE. In-depth analyses of the interactions between rivastigmine, the produced drug, and human acetylcholinesterase revealed that the compound interacts with just a few of the AChE catalytic active site residues, including a catalytic residue (His 447) and a crucial residue (Trp 86). The interaction with Tyr 337, which is absent in the produced molecule, is essential for the inhibition of the human enzyme.

Keywords: Pyrazolone, Acetylcholinesterase (AChE) inhibitors, Molecular docking.

Physicochemical properties and adsorptive capacities of sawdust-based biochars and commercial activated carbons towards ethoxylated alkylphenols from wastewater

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The quality of surface water, as well as of wastewater treated for its reuse, is increasingly compromised by the presence of organic micropollutants from both domestic and industrial origin. Within this latter category, ethoxylated alkylphenols with an alkyl chain length of eight or nine carbon atoms and an average number of ethoxylic units between three and ten, have been taken into consideration due to their large use and diffusion in the environment.

In this study biochar, obtained from waste biomass, was used as a sorbent medium of these organic compounds from a local wastewater treatment plant operating within a textile industrial district. The optimization of the inactivated production conditions of the adsorbent was evaluated based by nitrogen adsorption/desorption isotherms for the Brunauer–Emmett–Teller surface area, the t-plot microporosity and the Barrett-Joyner-Halenda mesoporosity. odine, phenol and methylene blue porosity indexes were also measured. The materials were also evaluated by elemental analysis, thermogravimetric analysis, pH of the point of zero charge, X-ray photoelectron and Fourier-transform infrared spectroscopy. Results showed the presence of surface aromatic domains and polar functionalities, together with a quite high surface area (320 m^2 g^{-1}), achieving a good sorption performances applying Langmuir and Freundlich isotherms. Considering the cheaper market price of biochar compared to activated carbons, which is at least 16 times less expensive, the management of the biomass waste by producing biochar can resolve important environmental, logistical and economic problems.

Key words: Biochar, Ethoxylated alkylphenols, Removal, industrial wastewater

EVALUATION OF CHEMICAL COMPATIBILITY BETWEEN TWO MIXED PRODUCED WATERS AND IDENTIFICATION OF MINERAL SCALE SAMPLE IN A SOUTHERN TUNISIAN OILFIELD

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Mineral scale formation is a serious flow assurance problem experienced in the oil and gas sector. It can cause not only flow reduction but also inefficiency and failure of production equipment. One of the primary causes of scale deposition is mixing two waters which are incompatible. In this case, predictive studies may help to evaluate the compatibility of the mixed waters and to prevent the scale formation, which usually occurs on rods, tubing or flow lines.

The purpose of this study is to evaluate the compatibility between two produced waters in a southern Tunisian oilfield, in order to identify the causes of scale deposition within the flowline of a comingled production.

Two water samples, "W1" and "W2", collected from the involved wells were analysed using inductively coupled plasma atomic emission spectroscopy ICP-AES, ion chromatography and other standard laboratory techniques. The results of complete waters analysis were the typical input parameters, to determine scaling tendency. Saturation indices values related to $CaCO_3$, $CaSO_4$, $BaSO_4$ and $SrSO_4$ scales were calculated for the water mixtures at different share, under various conditions of temperature, using a computerized scale prediction model.

The mineralogical characterisation of the scale samples collected from the flowline of the commingled production has been realized using XRD and SEM.

The compatibility study results showed that mixing the two waters tends to increase the probability of barite deposition. X-ray diffraction and SEM analyses confirmed the compatibility study results, since they proved that the analysed deposit predominantly consisted of barite.

At the studied temperatures conditions, the tendency for barite scale is significantly increasing with the increase of "W2" water share in the mixture.

The future scale inhibition and removal strategies to be implemented in the concerned oilfield are being derived in a large part from the results of the present.

Enhanced interfacial charge transfer by S-scheme in $Mn_{0.2}Cd_{0.8}S/CoFe_2O_4$ nano-composite for photocatalytic hydrogen production

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This study introduces an S-scheme mechanism for charge separation by coupling $Mn_{0.2}Cd_{0.8}S$ with $CoFe_2O_4$, alongside the incorporation of rGO as an electron mediator. To characterize the trinary $Mn_{0.2}Cd_{0.8}S/CoFe_2O_4$/rGO photocatalysts, we employed a range of characterization techniques, including X-ray diffraction, UV-Visible spectroscopy, Electrochemical impedance spectroscopy, Photoluminescence spectroscopy, and X-ray photoelectron spectroscopy. This approach opens promising possibilities for developing high-performance $CoFe_2O_4$-based photocatalysts for photocatalytic hydrogen production.

Key words: Ternary nanocomposite, reduced graphene oxide, hydrothermal method, photocatalytic hydrogen evolution

Synthesis, spectroscopic characterization, DFT calculation, of a new hybrid compound $(C_{11}H_{10}N)_2[ZnCl_4]$

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The crystallization and characterization of a new compound $(C_{11}H_{10}N)_2[ZnCl_4]$ by powder and single –crystal X-ray diffraction, thermal analysis DTA-TGA and X-ray micrography and microanalysis (SEM / EDX) are describes. A complete spectroscopic study has been carried out; it was accompanied by a comparative theoretical study, by DFT, carried out with Gaussian 09 software. The molecular unit of the compound is formed of two independent monoprotonated organic cations phenylpyridinium $(C_{11}H_{10}N)^+$ and an anion tetrachlorometallate(II), $[ZnCl_4]^{2-}$. The compound structure can be described as a succession of organic-inorganic layers parallel to the (001) plane. The cohesion and stability of these two materials are ensured by hydrogen bonds of the N-H…Cl type between the organic and inorganic layers as well as by van der Waals bonds. N-H…Cl type hydrogen bonds ensure the junction between the organic and inorganic layers leading to a three-dimensional arrangement 3D.

Hirshfeld's three-dimensional surface (3D-HS) and two-dimensional fingerprints (2D-FP) [1] reveal that the structure is dominated by Cl…H/H…Cl contacts; H…H and C…H/H…C. H…C.

Keywords: X-ray diffraction, fingerprints.

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Environmental friendly process at room temperature for the synthesis of MoO_2

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Molybdenum-containing materials play an important role in the technology sectors of today's growing industries due to its exotic electronic and physical properties, high melting point, hardness and chemical stability [1]. They are widely used in fabrication of electronic circuits, catalysts, lubricants, field emitters, sensing, electrochromic displays and energy storage applications. Among these, molybdenum oxides are technologically important materials because of its several applications in various electronic products due to their structural & electronic properties [2].

The MoO_2 crystalline state was revealed by X-ray diffraction (XRD). The analysis of Scanning electron microscopy (SEM) images reveals that the MoO_2 sample prepared is uniform with an average grain size of about 30 nm. The crystallite size has been carried by using various calculations methods such Scherrer, Williamson-Hall, and Size-Strain plot (SSP). Williamson-Hall (W-H) methods were used with: uniform deformation model (UDM), uniform stress deformation model (USDM) and uniform deformation energy density model (UDEDM) which were resulting important parameters such as stress (σ), lattice strain (ε), and energy density (u).

Key words: Nanomaterials, Crystal size, TEM, Strain

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Carbothermal synthesis of molybdenum (IV) oxide as a high rate anode for rechargeable lithium batteries.
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Preparation of MoO_2 sub-micro scale sheets and their optical properties.

Effect of nickel oxide and silica nanoparticles on glucose sensing and on electrical conductivity of a nanoporous carbon matrix

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In this work, we have studied the influence of nickel oxide (NiO) and silica (SiO_2) nanoparticles on the glucose detection capacity and on the variation of the electrical conductivity for the nanoporous organic matrix based on pyrogallol-formaldehyde (PF). Several characterization techniques were carried out on the different samples (PF matrix, PF:NiO and PF/SiO_2:NiO nanocomposites). The XRD diffractograms depict the appearance of broad diffraction peaks typical of both amorphous silica and carbon phases with the existence of three peaks of nickel in the two nanocomposites PF:NiO and PF/SiO_2:NiO. The SEM images show that the large number of particles covering the carbon matrix was observed in the PF/SiO_2:NiO nanocomposite. The TEM images indicate a significant porous texture of the PF matrix, a good dispersion of the nickel nanoparticles in the PF:NiO nanocomposite and an agglomeration of the nanoparticles in the PF/SiO_2:NiO nanocomposite. Electrochemical measurements show that the sensitivity of non-enzymatic glucose sensor increases with the decreasing of specific surface area. The electrical conductivity of these nanocomposites depends on the pore volume and it decreases with increasing this volume. The PF/SiO_2:NiO nanocomposite is very promising for electrochemical glucose sensor with sensitivity equal to 585 µA/mM.cm^{-2} and low electrical conductivity of around 10^{-8} Ω^{-1}.cm^{-1}.

Keywords: Carbon matrix; Porous materials; Nickel oxide; Silica; Non-enzymatic glucose sensor; Electrical conductivity.

Structural, Energy frameworks, Hirshfeld Surface analyses and electrochemical properties of alkaline earth-tetrazole coordination complexes.

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Alkaline earth-tetrazole complexes were synthesized through the in-situ transformation of the azide-nitrile cycloaddition reaction, utilizing alkaline earth (Ae) salts under hydrothermal conditions [1,2]. These compounds exhibit a complex three-dimensional hydrogen-bonded network, accompanied by pi-stacking interactions involving coordinated water molecules and tetrazole rings. The Hirshfeld Surface analysis, confirms the dominant role of C..N/N..C, N...H/N...H and N...N contacts in the crystal structure networks.

In addition, energy framework analyses were conducted on these compounds to examine the predominant effect of these interactions and hydrogen-bonding within the framework of the studied compounds.

Voltametric analysis of three synthesized complexes reveals quasi-reversible reduction waves attributed to the reduction of Ae^{+2}/Ae and irreversible reduction peaks corresponding to the ligand. Additionally, irreversible oxidation peaks are observed and assigned to the oxidation of the tetrazole rings.

Key words: Synthesis, Ae-Tetrazole, Coordination Complexes Electrochemistry. X-Ray Study, Hirshfeld Surface Analysis, Energy Frameworks analysis.

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Synthesis and Investigation of Physicochemical Properties of Two Novel Fluorescent Fluorenone Azine Derivatives: An Experimental and Theoretical Study

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In the pursuit of novel fluorescent capabilities, we synthesized two distinctive dyes; (E)-1-(2-hydroxybenzylidene)-2-(9H-fluoren-9-ylidene)hydrazine and (E)-1-(2-hydroxynaphtylidene)-2-(9H-fluoren-9-ylidene)hydrazine, denoted as (FIIS) and (FIIN), respectively. Their exploration unfolded through a meticulous analysis of photophysical attributes using electronic absorption and emission spectra within a DMF solution. Remarkably, the spectra revealed significant Stokes shifts ($\Delta\lambda > 80$ nm), suggesting promising prospects for these dyes in the specialized domain of biological fluorescence imaging. Delving into the electrochemical investigation, cyclic voltammetry provided insights within an Bu_4NBF_4 (0.1 M)/MeCN organic solution. Theoretical foundations were laid using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods, seamlessly aligning with experimental observations and establishing a theoretical scaffold for future investigations. These computational insights not only harmonized with experimental data but also enabled the computation of global reactivity descriptors for our synthesized molecules. Stepping into molecular interactions, our compounds displayed lower binding energy values (-7.3 and -8.4 kcal/mol) in comparison to the benchmark, kojic acid (-5.4 kcal/mol), suggesting potential inhibitory roles against tyrosinase activity. Expanding the scope, we scrutinized the absorption, distribution, metabolism, and excretion properties through screening both FIIS and FIIN against Lipinski's rule of five, employing the Swiss ADME server. Encouragingly, both molecules successfully met the specified criteria, fortifying the foundation for their potential applications.

Key words: Photophysical properties; Fluorenone azine; Cyclic voltammetry; DFT; TD-DFT; Molecular docking

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REVIEW OF GLUCOSE SENSORS' BASED ON ZNO MATERIAL

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Glucose is the most widely distributed and essential monosaccharide in nature. It has significant value in many fields, such as the food industry or material synthesis [1,2]. In human life and health, as an important energy source of cells, glucose has a vital impact on human health; ensuring the balance and stability of blood. Nowadays, diabetes, a chronic condition, is considered one of the deadliest and most rambling diseases globally. To overcome this challenging increase in diabetes, the scientific community makes enormous efforts to develop highly efficient, easily accessible and stable Glucose sensors to monitor the glucose level at the early stages of diabetes.

Objectives: The main goal of this research is to present the recent advances in the glucose sensor's service based on ZnO nanostructures. Some sensors can still maintain about 80% detection performance when they can be reused about 20 times. They optimize the catalytic efficiency of the reaction mechanism and provide potential ideas for improving the performance of other electrochemical Glucose sensors.

Methods: Among the numerous methods for detecting glucose concentration, ZnO-based electrochemical glucose sensors have shown great advantages such as good selectivity, highly sensitive performance and strong anti-interference ability. Indeed, Zinc oxide (ZnO) materials have attracted extensive attention in electrochemical sensing due to their wide bandgaps (3.32 eV) and high binding energies (60 MeV) [3].

The main advantages of ZnO-based electrochemical sensors is the good surface adsorption properties. And as a high-quality semiconductor material, ZnOcan provide an effective electron transport channel for based electrochemical glucose sensors.

Results: This review discusses the mechanisms of electrochemical glucose sensing with a focus on the different generations of enzymatic-based sensors, their recent advances, and provides an overview of the next generation of non-enzymatic sensors. Advancements in manufacturing techniques and materials are key in propelling the field of glucose sensing.

Due to health and regulatory pressures, the demand for low-cost, efficient, and accurate glucose sensors is significant, and the glucose market size is expected to be worth $36.7 billion by 2026 [4].

Keywords: enzymatic; non-enzymatic; glucose sensor; ZnO nanomaterial, electrochemical sensor

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Effect of magnetic and electrical properties in GaFeO3 with Zn, Ti co-doping

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Magnetic measurements, X-ray diffraction (XRD), as well as impedance analyzer are some of the techniques that have been employed in this study to evaluate how the dielectric, magnetic and structural properties of $GaFeO_3$(GFO) ceramics are affected by Ti and Zn doping. polycrystalline $Ga_{1-x}Zn_xFe_{1-x}Ti_xO_3$ ($0 \leq \times \leq 0.1$) were prepared by solid state reaction. They showed an orthorhombic crystal structure with $Pc2_1n$ space group. The magnetic transition temperature decreases due to the dilution of the magnetic interaction. A noteworthy effect of substitution of multiple elements at the Ga and Fe sites on dielectric constant and tangent loss of $GaFeO_3$ has been observed. Complete studies of temperature and frequency dependence of dielectric constant and impedance have provided the effect of grains and grain boundaries on the conduction mechanism and dielectric relaxation of the material. Impedance spectroscopy results have revealed a distinct conduction process at grain and grain boundaries.

Keywords: Multiferroic; material Mossbauer; analysis Magnetism Site disorder; Dielectric study

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Stable Al(III) complexes of a water-soluble Schiff base: Overcoming hydrolysis for improved water stability

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Aluminum, the most abundant metal in the Earth's crust and a biological non-essential element, is widely used in industry and daily life in applications such as water treatment systems, food additives, cosmetics, packaging materials, and pharmaceutical drugs.

Although the *N*,*N*′-ethylenebis(salicylimine) (salen) chelating double Schiff base ligand and its derivatives are probably amongst the most extensively investigated ligands, there is an increasing demand to use metal-salen complexes in aqueous systems due to the current upswing in aqueous organometallic catalysis. However, this is frequently hampered by the complexes' insolubility in water. Therefore, we optimized the synthetic conditions and obtained a water-soluble Schiff base *N*,*N'*-bis(3-methoxyl-5-sulfonatosalicylidene)-1,2-ethylenediamine disodium salt (abbreviated as MSS), prepared by condensing 3-methoxyl-salicylaldehyde-5-sulfonate sodium and 1,2-ethylenediamine. Special attention was given to the investigation of the phenol-imine (O-H···N) // keto-amine (O···H-N) equilibrium of MSS in solutions of different solvents. The Schiff base ligand MSS was then employed in complexation studies in aqueous solution and to synthesize novel Al(III) complexes in non-aqueous media. All the studied compounds were investigated by carrying out NMR, UV/vis and ATR-FTIR spectroscopies, complemented with density functional theory (DFT) and time-dependent DFT calculations.

Strategies to reduce the dissemination of antibiotic resistance in the environment

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Antibiotics are widely used in veterinary practice especially in poultry production for the prevention and treatment of bacterial infections and as growth promoters [1]. Based on their chemical structure and mechanism, antibiotics can be divided into different categories, namely ß-lactams, sulphonamides, quinolones, tetracyclines, macrolides, aminoglycosides, etc [2]. However, due to low adsorption and incomplete metabolism of antibiotics by animals treated with, much of it is excreted through urine and feces as unchanged main compounds into the environment [3]. As a result, antibiotic residues are often detected in surface water, groundwater and even drinking water, causing severe health problems in humans and animals because of their toxic effects and long half-lives [4]. Besides, the widespread use of antibiotics has led to the problem of the development of bacterial antibiotic resistance [5]. Therefore, it is of great importance to develop effective methods to eliminate antibiotics from wastewater, thereby reducing the emergence and spread of antibiotic resistant bacteria (ARB). The aim of this study is to synthesize biobased polymers as synthetic adsorbent phases to remove antibiotics and their residues from poultry farm effluents, in order to limit the selection and the dissemination of antimicrobial resistance from chicken production to the environment, and ultimately to humans.

Key words: antimicrobial resistance, antibiotics, biobased polymers, adsorption

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Design of partially biobased polymers with triazine groups for adsorption of polyphenols

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Phenolic compounds present a particular challenge, as they are likely to persist in the environment for long periods, accumulating and producing toxic effects for both humans and animals. To minimize the effects of these compounds, several techniques have been used to eliminate them. Among these, adsorption is considered one of the most effective and widely used methods, thanks to its ease of application, low cost, high efficiency and regenerative capacity. To this end, a series of polymers (P1-P6) were synthesized by polycondensation with different monomers of biological origin. These polymers were characterized by NMR spectroscopy, differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The polymers studied were tested as solid phase adsorbents for phenolic compounds in water. Adsorption results showed that the biosourced polymer P2 exhibited superior adsorption efficiency for all target aromatic compounds (polar and non-polar molecules). We also concluded that incorporation of the triazine group into the polymer chemical structure has a major effect on increasing adsorption efficiency.

Keywords: phenolic compounds, polyphenols, bio-based monomer, polymers, adsorption

Developing Molecularly Imprinted Polyaniline-Carbon Paste Electrodes for an Electrochemical Sensor to Detect Oxytetracycline in Real Sample

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Oxytetracycline (OTC), a type of pharmaceutical and personal care product (PPCP), is widely utilized as a broad-spectrum antibiotic for disease prevention, infection treatment, and as an additive in livestock farming. Due to their extensive use in aquaculture and the agricultural industry, both the unaltered parent compounds and their metabolized products have been commonly found in surface water, groundwater, and sewage treatment plants. These substances can be absorbed by humans through the animals treated with these drugs, posing a serious threat to human health, including allergies, toxic effects, and bacterial resistance. Hence, developing an effective detection method for OTC compounds is of paramount importance. Addressing the analytical challenge, electrochemical sensing employing molecularly imprinted polymers (MIPs) has emerged as a crucial technique in environmental monitoring due to their superior chemical and physical stability, cost-effectiveness, high selectivity, and rapid response. Significantly, constructing MIP sensors involves leveraging low-cost bioadsorbents such as Posidonia to achieve heightened sensitivity. This study focuses on developing MIP@POS, using polyaniline (PANI) polymer, for the detection of OTC. The materials were created through copolymerization, attaching aniline to the surface of Posidonia along with free aniline to form a chemically bound thin layer of PANI on the Posidonia surface. The obtained MIP@POS was characterized using various analyses, including pHPZC determination, and analysis techniques (FTIR, 13C CP-MAS NMR, SEM, and TGA). The electrochemical analysis of OTC involved a glassy carbon electrode (GCE) modified through an electrochemical pre-treatment method in an acidic medium. For all the investigated OTC, distinct irreversible cyclic voltammograms for the oxidation of OTC antibiotics exhibited the highest current signals at 0.9V versus Ag/AgCl in a 0.1M phosphate buffer solution (pH 6) with a scan rate of 100mV/s, compared to the bare glassy carbon electrodes. Linear calibrations were achieved ranging from 0.5 to 50µM for OTC. The voltammetry conditions, including scan rate, pH, deposition potential, and deposition time, were systematically optimized. Lastly, the MIP@POS-carbon paste electrode was prepared using the 'Latex' method for direct application to real samples.

Keywords: Oxytetracycline (OTC), Posidonia, Polyaniline, Molecularly imprinted polymer (MIP), electrochemical sensor, cyclic voltammetry.

Green resins without formaldheyde from Organosolv lignin and Tannin

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Organosolv lignin from Alfa grass mixed with Aleppo pine tannin and glyoxal as hardner were used as wood adhesive resins in particleboards fabrication and porous areogel materiel. The condensed tannins extracted from Aleppo pine bark roots was examined in near industrial conditions, using a water medium in presence of 2% NaHCO3, 0.5% NaHSO3 at 70°C. The tannins extracts were recovered in high yields (~25% of Aleppo pine with high phenolic contents (>75%). The tannins were characterized by ^{13}C NMR and MALDI TOF and shown characteristics of procyanidin/prodelphinidin units. Adhesive resin formulations were prepared using Aleppo tannins and cross linker such as glyoxal. The resins were studied by TMA in bending and tannins-based formaldehyde-free wood particleboards were produced. The panels displayed very good internal bond strengths with the four hardeners and all of them passed relevant international standard specifications for interior-grade panels. The best results were observed with the tannins extracted at 70°C with furfural as hardener (IB = 0.81MPa for Aleppo pine and IB=0.76 MPa for sumac).

Porous organic aerogels have been prepared using sumac tannins and three different cross linkers (glutaraldehyde, furfural and glyoxal) and NaOH as a basic catalyst. A few formulation of hydrogels were obtained to reproducible hydrogels which were subsequently supercritically dried. A broad family of aerogels was thus obtained. These materials were investigated in terms of porous structure, based on pycnometry, adsorption and electron microscopy studies

Keywords: Alfa grass.; tannin; lignin; organosolv; Lewis acid; mosoporous material, glyoxal.

Supramolecular association of (*p*-xylylenediaminium) bis(perchlorate) monohydrate: A Combined Experimental and Theoretical Study

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The crystal structure of the new material (*p*-xylylenediaminium) bis(perchlorate) monohydrate, $(C_8H_{14}N_2)(ClO_4)_2.H_2O$ that was prepared in crystalline form by solvent evaporation method at room temperature. Single crystal X-ray diffraction analysis shows that this compound crystallizes in the monoclinic system, with the space group $P2_1/c$. The title structure benefits from extensive intermolecular interactions such as C-H… π interactions and hydrogen bonds which are the major forces to make it more stable in the solid-state. The interactions in the solid-state have been also studied using Hirshfeld surface analysis (d_{norm}, curvedness, and shape index), as well as its 2D fingerprint plots. To reinforce experimental results, DFT calculations have been performed via the B3LYP method with 6–311++G (d,p) basis set. HOMO-LUMO energies and the chemical quantum descriptors were taken into account. Atom In Molecules (AIM) and Reduced Density Gradient (RDG) analyses have been explored to reveal the steadiness of the molecule. Molecular electrostatic potential inspection has also been submitted in the study. Finally molecular docking studies show that the synthesized compound may act as potential acethylcholinesterase inhibitor.

Keywords: Crystal structure, DFT calculations, Hirshfeld surface, Vibrational study, AIM, Molecular Docking.

Synthesis, Structure and Photoluminescence Properties of 0D Hybrid Tin(IV) Halide Perovskites-Like: $[Cl\text{-}(CH_2)_2\text{-}NH_3]_2SnX_6$ (X=Cl; Br)

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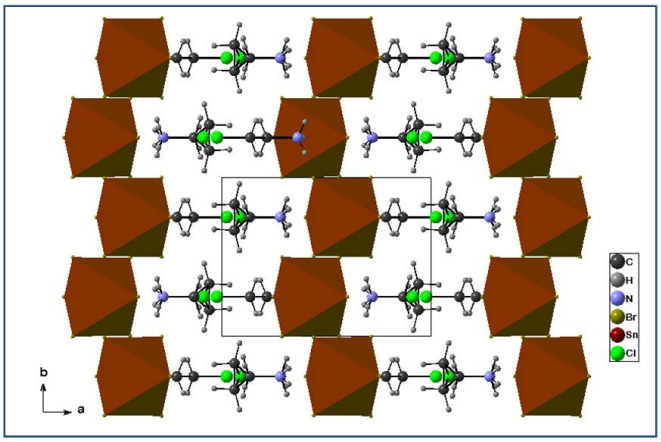
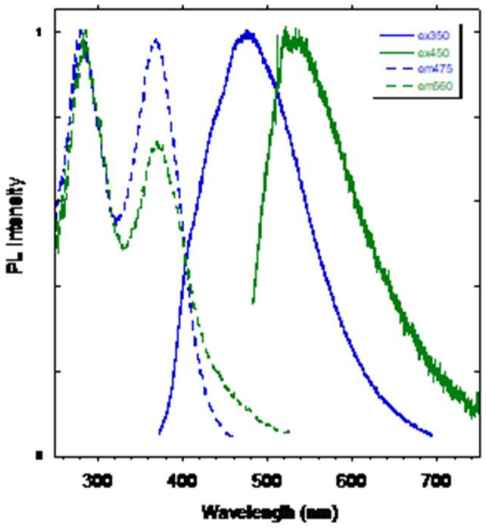
Low-dimensional hybrid perovskites are an emerging class of materials with high stability and excellent optoelectronic properties. Herein, we introduce two novel, lead-free, 0D perovskite-like materials, (2-chloroethylammonium)$_2SnX_6$ (X=Cl; Br), for luminescence applications. Single-crystal X-ray diffraction analysis revealed a perovskite-derivative structure having the inorganic SnX_6 periodically arranged in the crystallographic *a*-axis and sandwiched by independent layers of organic cations. Their crystal structure and surface morphology were studied. The effects of different halogens and organic amines on perovskites' emission spectra were investigated, and the photoluminescence (PL) properties were studied. This finding may pave the way for new 0D hybrid materials with targeted properties.





Keywords: Lead-free, Hybrid perovskites, Crystal structure, (PL) properties, Optoelectronic properties.

Valorization of a natural bio-flocculant and optimization of COD removal from wastewater treated by electrocoagulation: Application of Box-Behnken design

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In this work, we used a new biodegradable organic flocculating agent we extracted from the Mesembryanthemum crystallinum, in a physicochemical process (coagulation- flocculation) and in the electrocoagulation/electro flocculation process order to treat liquid rejections industrial.

This bio-flocculent helps reduce the turbidity of industrial effluents, making it pass from 1119 NTU to values below 120 NTU, the use of glacial flocculent as a coagulant also allowed the reduction of COD from 924 to 80. mg/L O2

The tests were carried out on pseudo-industrial samples prepared at the laboratory and samples from a surface treatment unit. The comparative study of the organic flocculating agent with the industrial flocculating agent, Aluminum sulfate, showed the bioflocculent's very good competitiveness and its strong capacity of flocculation. Neutralization and coagulation with lime, followed by flocculation then decantation, for water waste, showed a very significant effect on the abatement of turbidity and, the "Chemical Oxygen Demand" (COD).is work brings to satisfactory results which incite our team to further research in order to boost our national natural resources by using alternate proper processes for water treatment.

Keywords: Industrial effluent, Mesembryanthemum crystallinum, turbidity, bio-flocculating agent, treatment, electro coagulation- electro flocculation.

Evaluation of physical, chemical and microstructural properties of biomaterials based on nopal cactus

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In this work, Opuntia ficus indica were first characterized and then valorized according to two different approaches: (i) a simple pyrolysis to make activated charcoal and (ii) a use after a chemical extraction of mucilages to different pH values for microcapsule synthesis. Indeed, a study concerning the characterization of mucilaginous extracts was carried out using several methods and techniques. Fourier transform infrared spectroscopic analyzes of the mucilages revealed the presence of galactose and pectin. Scanning electron microscopy (SEM) revealed that most of the particles adhered together and caused the formation of compact bound agglomerates, which gave different irregularly shaped microstructures. The mucilaginous extracts resulted in encapsulation with a narrow size distribution and diameters ranging from 4 to 12 µm and encapsulation efficiency ranged from 83% to 87%. These results confirmed the deposition of coacervate droplets around the oil drops and clearly showed that the formation of coacervated particles and their deposition on the oil droplets were successive events, in particular via a complex coacervation. In the first approach, the dried cuttings of the trunk of the barbaric fig tree were converted into activated charcoal for the retention of p-nitrophenol. A kinetic adsorption study was carried out and showed that the adsorption equilibrium was reached after 120 min, following a pseudo-second-order model. The study of adsorption isotherms revealed that the Langmuir linear model is the most credible model to describe the adsorption of pNP, and has a maximum adsorption capacity of 16.83 mg / g. After some saturation, the activated carbon was regenerated effectively by washing with NaOH solution. To conclude, both approaches have yielded materials with promising properties, which presents a viable option for rational recovery of abundant industrial waste from a renewable source.

Keywords: Opuntia ficus indica, activated charcoal, microcapsule.

Crystal structures of a new supramolecular Chloroantimonate(III) Hybrid materiel with α-Methylbenzylaminium : Vibrational studies, Thermal Properties, Opto-electric properties and atomic Hirshfeld surface analysis.

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The title compound $(C_8H_{12}N)_4[SbCl_5]_2$ was obtained at room temperature by slow evaporation in the centrosymmetric triclinic space group $\mathbf{P2_1/c}$ with the following parameters: a = 29.0349(16) Å, b = 13.1241(7) Å, c = 12.0278(7) Å, β = 95.567(2) ° Z = 2 and V = 4561.7(4) Å^3. The asymmetric unit consists of two independent $[SbCl_5]^{2-}$ anions and four protonated cations $(C_8H_{12}N)^+$. The cavities between the inorganic entities were occupied by organic cations to ensuring their connection by the means of N—H…Cl hydrogen-bonding interactions leads to the formation of a three-dimensional network. The infrared IR and Raman studies which were recorded at room temperature charge in the 4000-400 cm $^{-1}$ and 0-4000 cm $^{-1}$ frequency regions, respectively, confirmed the existence of vibrational modes that correspond to the organic and inorganic groups. Hirshfeld analysis results shows that predominate interactions were H…Cl. The Thermogravimetric analysis (TGA) shows that the compound remains stable up to about 150°C. The optical properties were characterized experimentally by UV-Visible absorption studies and photoluminescence measurement.

Experimental and theoretical investigations of the solid state photophysical properties of some N-Substituted iminocoumarins

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Coumarins dyes are well known being one of the most intensively studied organic materials mainly due to their interesting photophysical properties. Indeed, their optical properties have been recently reported by several combined experimental and theoretical studies. Mainly, their 2-iminocoumarin analogues exhibited very remarkable optical properties although the very few related reports. Interestingly, they have attracted great attention thanks to their high fluorescence capacity, and their relatively high quantum efficiency. This interest is essentially due to the strong alteration and dependence of their photophysical properties on the nature and position of the substituants. They therefore have been widely used in many optoelectronic applications such as DSSCs solar cells [1], fluorescent sensors [2] and lasers [3].
Under the motivation mentioned above, we will present, in this work, experimental and theoretical investigations of the photophysical properties of iminocoumarins carrying a free imino group and their N-substituted analogues at the solid-state level. We will extract the substitution effects on the light absorption and emission characteristics. Good agreement between experimental and theoretical findings was provided [4].

Key words: Iminocoumarins, Substitution, Optical absorption, Fluorescence, DFT - TDDFT

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Thermogravimetric Kinetic Analysis of the pyrolysis of Tunisian Juniper needles

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A kinetic of the pyrolysis of juniper needles is investigated with thermogravimetric analyzer TGA with non-isothermal methods selected for analyzing solid-state kinetics data is presented. The mass loss was measured by TGA in nitrogen atmosphere. The samples were heated over a range of temperature from 298 K to 1073 K with four different heating rates of 5, 10 and 15 and 20 K min^{-1}. Thermogravimetric analysis showed three distinct zones of thermal decomposition: cellulose, hemicellulose and lignin. Two model-free (isoconversional) methods, Kissinger-Akahira-Sunose (KAS) and Flinn-Wall-Ozawa (FWO) were used to determine the apparent activation energy. Activation energy average values were shown to be 186.91-180.19 kJ mol^{-1} as calculated by KAS and FWO methods, respectively.

Keywords: kinetic, pyrolysis, thermogravimetric analysis (TGA), activation energy

Preparation and characterization of two compounds in Na_2O-CoO-X_2O_5 (X: As, P) systems.

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In the context of this presentation, we have prepared a series of solid solutions in the Na_2O-CoO-X_2O_5 (X = As, P) systems. From these formulations, we successfully synthesized two distinct phases $Na_4Co_7(PO_4)_6$ and $Na_4Co_7(AsO_4)_{1.5}(PO_4)_{4.5}$. Furthermore, the structural aspects of these compounds were elucidated through a combination of Raman and IR spectroscopies identifying functional and molecular groups by analyzing their vibrational modes. The investigation also employed X-ray diffraction (XRD) to resolve the polycrystal structure and scanning electron microscopy (SEM) for detailed morphological analysis. Finally, electrical measurements were conducted on both compounds. The comprehensive set of results obtained from these various analyses constitutes the focal point of this presentation.

Mots clés : DRX, phosphate, ionic conductivity, solid- state method.

Crystal Structure, thermal study, vibrational and optical properties of a novel dinuclear Bismth(III) Iodide trimethylenedipyridine compound

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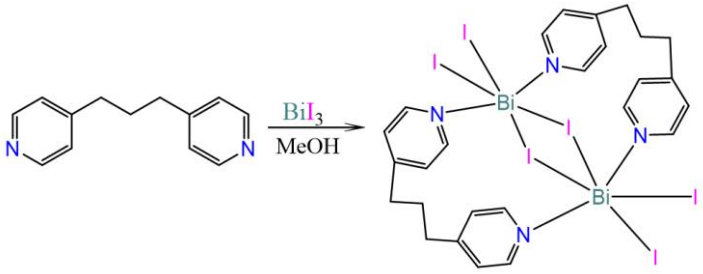
Bismuth-based materials have stimulated much interest due to their unique photoluminescence behavior. To date, several luminescent bismuth (III) complexes ligated by *N*-donor ligands have been investigated [1-3]. In this work, a new luminescent binuclear compound built from BiI_3 with a pyridine-type ligand, synthesized in MeOH solution and crystallized under slow evaporation method. This halide-bridged binuclear compound, which is also doubly bridged by 4,4'-trimethylenedipyridine, was characterized through single crystal X-ray diffraction at 100 K. Its thermal behavior was investigated via TGA-DTA, as well as its vibrational spectra by Infrared and Raman spectroscopy. Furthermore, the photoluminescence properties were examined through steady-state and time-dependent luminescence techniques.



Schema: Synthesis of Complex

Key words: Bismuth halide, N-donor ligand, luminescence, X-ray diffraction.

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DFT study of a gas detector based on the Gr/ZnO heterostructure

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Zinc oxide (ZnO) is a material with a wide range of commercial uses specifically in gas sensors. Although ZnO has been extensively researched for gas detection, gas adsorption by ZnO polar surfaces is the subject of very few publications. In this work, we evaluate the performance of Gr/ZnO polar surfaces heterostructure for NH3 and NO2 gas detection.

The thermoelectric properties of ZnO polar surfaces verified the important electrical conductivity of these surfaces and showed their metallic behavior.

We have examined ZnO polar surface relaxation and surface energies. Since the O-polar surface was more stable, we continued our study evaluating the adsorption of NH3 and NO2 gases by the ZnO O-polar surface and Gr/ZnO O-polar structure. Different adsorption sites were studied.

The ab initio calculation was carried out within the framework of density functional theory (DFT). We have examined Gr/ZnO(000-1) structure relaxation, binding energies, and the band structure and density of states of the stable structures of NO2 and NH3 adsorbed on Gr/ZnO(000-1).

The density of states shows that the contribution of the NH3 molecule adsorbed on Gr/ZnO appeared in the valence band for deep energy levels, and the adsorption of the NO2 molecule occurs through interaction between the p orbitals of oxygen atoms of NO2 molecule and oxygen atoms of ZnO surface.

Key words: Graphene, zinc oxide, density functional theory, electrical conductivity, gas sensor, ammonia, nitrogen dioxide.

An Electrochemical Sensor for Sulfadiazine Determination Based on a Copper Nanoparticles/Molecularly Imprinted Overoxidized Polypyrrole Composite

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An electrochemical sensor for sulfadiazine detection based on molecular imprinted polymer film is described in this work. This sensor was prepared by electro-polymerization using pyrrole as a functional monomer and sulfadiazine as template onto the surface of copper nanoparticles-modified glassy carbon (GC) electrode. The electrochemical behaviour of the imprinted and nonimprinted polymer (NIP) was carried out by differential pulse voltammetry (DPV)

Throughout this study various analytical parameters, such as pH value, concentration of monomer and template, impact of scan rate and electro-polymerization cycles were investigated and optimized. Under the optimized conditions, the peak current of sulfadiazine was linear to its concentration in the range of 10^{-9} -10^{-5} mol L^{-1} with a detection limit of 3,1 x 10^{-10} mol L^{-1}. Additionally, this sensor exhibited an excellent selectivity even in the presence of molecules with similar chemical structures.

Keywords : Sulfadiazine, molecular imprinted polymer, pyrrole, copper nanoparticles

Effects of experimental conditions on properties of polyaniline thin films obtained by Polymerization/Nucleation method

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We prepared thin films of polyaniline doped by HCl and deposited on glass substrates at various experimental conditions by using the technique of simultaneous polymerization/nucleation. We studied the effect of temperature and the duration of the polymerization reaction on film characteristics. We prepared films at 0°C and 25°C for various reaction times: from 1 min to 20 min. films were characterized by Uv-Vis absorption, FTIR and DRX. Films prepared at 0°C showed better homogeneity and higher surface quality for the time reaction not exceeding 10 min. FTIR measurements showed the characteristic absorption bands of polyaniline. By DRX we showed the semi-crystalline structure of the polymer in Emeraldine salt form and an amorphous structure in its Emeraldine base form. From Uv-Vis absorption measurements we obtain the energy gap Eg, around 1.5 eV and we find that Eg depends on solvent and temperature reaction. This value is compatible with the semiconducting nature of this polymer.

Key words: Polymerization, Conducting Polymers, Thin films, Nucleation, Semiconductors

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Characterization of Microstructure, Exchange Interaction, and Magnetism in Nanocrystalline Zr_6Co_{23}/MgO(001) Films

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In this study, we explored the influence of thickness (δ) on both the microstructural and magnetic characteristics of nanocrystalline Zr_6Co_{23} films grown on an MgO(001) substrate. A series of Zr_6Co_{23}/MgO(001) films were systematically prepared with varying thicknesses (δ). The coercivity (H_c), squareness factor (S*), and anisotropy field (H_a) were investigated in relation to δ thickness and grain sizes (Φ). Remarkably favorable magnetic properties were observed for δ = 100 nm, featuring a coercivity of H_c = 3020 Oe, a maximum energy product ($(BH)_{max}$) of 28 MGOe, and a magnetic anisotropy constant (K_1) of approximately 1.35×10^7 erg/cm^3. The study delves into the interconnections among exchange interaction, magnetic domain structure, and anisotropy parameters. These findings serve as a foundational reference, offering insights to tailor the magnetic properties of Zr_6Co_{23}/MgO(001) films for potential applications in the realm of permanent magnets [1].

Key words: Microstructure, Magnetic Properties, Zr_6Co_{23}/MgO(001) Thin Films, Ferromagnetic resonance.

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Effect of the drying process on the textural and structural properties of elaborated TiO_2

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In recent years, high concerns have been raised about atmospheric environmentally hazardous wastes. In particular, the release of chlorinated volatile organic compounds (Cl-VOCs) has received much attention due to the major health problems associated with the exposure to these compounds. Supported vanadium oxide is reported as a very active catalyst resistant against chlorine poisoning. In particular, TiO_2 anatase, as a support for the V_2O_5 active phase, is receiving great attention due to its good mechanical, thermal, and anticorrosive properties. Indeed, synthesizing anatase TiO_2 with high surface area is a key in the development of efficient catalysts.

In this work, we were interested in the effect of the drying process on the textural and structural properties of elaborated TiO_2. The synthesis of TiO_2 supports was carried out as follows: first, titanium (IV) isopropoxide as precursor with anhydrous ethanol as solvent was chemically modified by adding acetylacetone to control hydrolysis and condensation reaction rates. A homogeneous gel is then obtained after HNO_3 supply. Water is added according to the molar ratio $h=H_2O/Ti$ equal to 5, 7.5 and 10 in order to investigate the effect of the hydrolysis ratio on the surface area of TiO_2.The obtained gels were, thereafter, transformed either into aerogels by supercritical drying (P= 63 bar, T= 243 °C) or into xerogels by oven drying. The materials were then calcined for 12 h at 500 °C under O_2 flow (30 ml/min).

According to XRD patterns, all solids (aerogels and xerogels) show only diffraction lines due to TiO_2 anatase. However, these lines are more accentuated in the case of aerogel materials. In the other hand, the xerogel maerials was found to display lower BET surface areas compared to those of aerogels which develop similar BET surfaces (around 100 m^2/g). In addition, the average pore diameter is larger in the case of aerogels for all hydrolysis ratios tested, while the porous distribution is better when h=10 or 5.

Key words: TiO_2, aerogel, xeogel

Role of Sn atoms on Pd(1 1 1) and Pt(111) surface in reduction of hydrogen peroxide: DFT calculations

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In this work, we studied the effect of the addition of Sn atoms on Pt(111) and Pd(111) in the reduction of hydrogen peroxide by applying the grand-canonical DFT to explicitly take into account the effect of the electrochemical potential. We report the results of modeling the hydrogen peroxide reduction (HPRR) to H_2O on Pt_2Sn(111)/Pt(111) and Pd_2Sn(111)/Pd(111) surfaces at different applied potentials using (GC-DFT), a method specifically designed to model electrochemical systems.

The aqueous electrolyte is taken into account using an implicit solvent model, and the dependence of the reaction energetics on the electrode potential is derived using GC-DFT. Compared to pure Pd(111) and Pt(111), the adsorption of the HPRR intermediates are weakened on the Pt_2Sn(111)/Pt(111) and Pd_2Sn(111)/Pd(111) surfaces. The rate determining step is $OH + H^+ + e^- \rightarrow H_2O$ on Pt_2Sn(111)/Pt(111) and Pd_2Sn(111)/Pd(111) and pure Pd(111), $H_2O_2 \rightarrow OH + OH$ on pure Pt (111). Compared to the energy barrier of the rate-determining step on pure Pt(111) (0.35eV) and Pd(111) (0.6 eV), the activity of the HPRR reaction degrades on the Pt_2Sn(111)/Pt(111) and is hindered on Pd_2Sn(111)/Pd(111), with barriers of 0.85 and 0.80 eV, respectively at 0.6 V/ENH. The potential for occurrence of experimental H_2O_2 reduction is in good agreement with the thermodynamically favorable potential for adsorption of $H^+ + 1e^-$ on the surface. The reduction onset potentials of Pt_2Sn(111)/Pt(111) and Pd_2Sn(111)/Pd(111) should be 0.4 and 0.55 V, respectively. Among the studied surfaces, the addition of Sn on a Pt(111) surface shows the highest reactivity and is more active than on Pd(111). We believe that the adsorption of H on the surface determines the overvoltage.

EPR and magnetic study of two copper complexes $[Cu(C_6H_9NBr)_2(NO_3)_2]$

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In this work, a magnetic study of two copper complexes was developed, the T-dependent magnetization shows (μ_{eff} = 1.98 μ_B for **CuL^1** and 2.00 μ_B for **CuL^2** with 2-bromo-5-methylpyridine (L1) and 2-bromo-4-methylpyridine (L2)) and it shows also very small Curie-Weiss constants of about –1. The EPR spectra of both complexes show axial symmetry, very similar averaged *g* values of 2.123 and 2.125, respectively and no hyper-fine splitting in line with their tetragonally elongated octahedral structures. A Curie-Weiss fit of the inverse magnetic susceptibility yields nearly identical effective magnetic moments of μ_{eff}. The effective moments larger than the spin-only value of 1.75 μ_B expected for a $3d^9$ configuration (S = 1/2) indicate spin-orbit coupling.

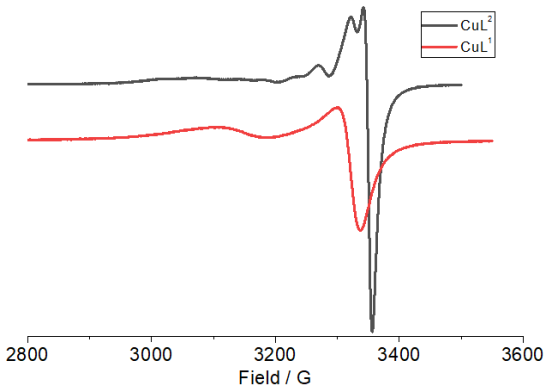

Figure: *X-band EPR spectra of the two Cu(II) complexes $[Cu(L)_2(NO_3)_2]$.*

Key words: Copper, Curie-Weiss, EPR.

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Synthesis, physico-chemical characterization and crystallochemical study of a new zero-dimensional (0D) hybrid pervoskite phase $(C_5H_6BrN_2)_2[CuCl_4]$

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In this work we reported the synthesis, the physico-chemical properties and the crystallochemical study of a new 0D hybrid perovskite phase of formula $(C_5H_6BrN_2)_2[CuCl_4]$. Various experimental techniques were used for the physico-chemical characterizations of the compound prepared: powder and single crystal X-ray diffraction and spectroscopic studies (IR, Raman, liquid and solid UV-visible, diffuse reflectance and photoluminescence). Powder X-ray diffraction analysis confirmed the purity of the synthesized phase. The study by infrared and Raman absorption spectroscopy allowed us to determine the vibrational characteristics of the elaborated phase and specially to ensure the protonation of the amine used. UV-visible absorption spectroscopy, diffuse reflectance and photoluminescence were used to measure the optical properties, showing that this compound has semiconducting properties. In addition, the single crystal X-ray diffraction study showed that the compound $(C_5H_6BrN_2)_2[CuCl_4]$ crystallizes in the monoclinic system with a centrosymmetric *C*2/c space group. The structural data of this compound reflect the formation of a distorted tetrahedral geometry around Cu (II). Its structure can be described as an arrangement of organic layers located at *z*= 0 and *z*=1/2, formed by $(C_5H_6BrN_2)^+$ cations, alternated with inorganic layers located at *z*= 1/4 and *z*=3/4, formed by chlorocuprate anions $[CuCl_4]^{2-}$. These two types of layers are parallel to the (001) plane and linked together by N-H···Cl hydrogen bonds to form a three-dimensional network. Hirshfeld surface analysis confirms that N-H···Cl hydrogen bonds play an important role in the stabilization and cohesion of the crystal structure.

Key words: crystal structure, 0D hybrid perovskite, cholorocuprate(II), optical properties

OPTIMIZATION OF A LOW COST CEMENT MORTAR BY DOEHLERT EXPERIMENTAL DESIGN

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As part of the circular economy, the cement industry plans to partially replace cement powder with alternative materials such as industrial waste, more particularly complementary cementitious materials of a mineral nature such as silica fume, fly ash which are rich in pozzolans (Silica) with well-defined percentages of lime (CaO) which are basic constituents to establish the pozzolanic reaction which gives rise to hydrated calcium silicates (CSH) responsible for the rigidity of the cement developed. In this work, other types of waste have been incorporated such as industrial waste (glass waste), also food waste (egg shells) and biosourced materials (Posidonia fiber). The main objective is the development of an ecological cement respectful of the environment with improvement of these mechanical performances. In this study, we succeeded by using a response surface methodology (Doehlert Design) in developing a cement having a mechanical compression strength of 33.2 MPa and flexure mechanical strength of 5.39 MPa compared to the control Portland cement and this following a substitution of 9.28% of the cement powder by three types of waste (glass powder, posidonia fiber and eggshells).

The optimal composition was characterized from thermal properties and gave after 28 days a conductivity of 1.81 W/mK and a diffusivity of 1.3 mm^2/s which is encouraging for a new semi-ecological cement.

Keywords: Portland Cement, semi ecological, Doehlert design, compressive strength, flexure strength, thermal properties.

Preparation and characterization of an activated carbon based on orange peel

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Activated carbon is widely used in energy storage applications, particularly in the field of electrochemical energy storage devices. It has also several potential applications. This study focuses on the effectiveness of activated orange peel as an absorbent material for the removal of methylene blue dye in an aqueous environment. The uses of activated carbon in other applications are explained in details. The preparation and characterization of the material are achieved in the following order: preparation of orange peel using a standard protocol. Then, the analysis of the obtained material is achieved by SEM, IR and UV. The material capacity is measured by the use of methylene blue concentration gradient. The results revealed that the prepared material is a promising, economical and environmentally friendly potential for several uses such as: energy storage, contaminated water treatment and so on.

Key words: activated carbon, orange peel, adsorption, storage energy, water treatment.

Effects of mechanical alloying on microstructural changes of Al-Ni-Zr compound

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The mixtures of Al, Ni and Zr elemental powders with nominal composition Al90-Ni7-Zr3 at.% was mechanically alloyed in a planetary ball mill under argon atmosphere. The structural and morphological changes during high-energy mechanical alloying were investigated by X-ray diffraction and scanning electron microscopy. We have found differences in the kinetics of solid-state reactions. This difference was attributed to the state and reactivity of the different precursors and the properties of phases formed during milling. The final products of the mechanical alloying process were nanocrystalline aluminiuml-rich solid solutions with a mean crystallite sizes in the range of a few nanometers. As a result, the prolonged milling time allows the disordered Ni_3(Al,Zr) solid solution to dissociate to the Al(Ni,Zr) phase and Al(Ni)) phase.

Calorimetric studies demonstrate the coexistence of overlapping exothermic peaks characteristic of crystallization processes associated with the identified phases.

Key words: Nanostructured materials, Mechanical alloying, X-ray diffraction, Phase transformation, Thermal analysis

Effect of synthesized organic copolymers containing both carboxylate and hydroxyl groups on aqueous alumina dispersion

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Copolymers containing both carboxylate and hydroxyl groups noted PV2A have been synthesized in order to act simultaneously as dispersant and binder for spray drying alumina suspension. The quantity of the added copolymer was optimized to achieve adequate dispersion and stabilization of the suspension. Such investigation was done through a systematic analysis of the electrokinetic and rheological properties, from which the copolymer /alumina interactions during the powder dispersion can be evaluated. The addition of 1.2wt % of the PV2A copolymer in the formulation of an alumina suspension provides good stability, with a quasi-Newtonian rheological behavior and a minimum viscosity of 25 mPa.s.

Adsorption isotherm provided an electrosteric stabilization of alumina suspension, promoted by the adsorption of carboxylic groups onto the alumina surface and a loop-like conformation of hydroxyl groups.

The effect of polymeric chain length on the dispersion was studied using three copolymers $PV2A_L$, $PV2A_M$, $PV2A_H$ having respectively low, medium and high molecular weights estimated to 11,000, 19,000 and 47,000 Da. The strong attraction between dispersant and binding groups in the polymeric chains of PV2A prevents the competitive adsorption onto the alumina surface, usually obtained with commercial organic additives. As a result, the phenomenon of binder migration was prevented during the spray-drying, leading to a homogenous microstructure of atomized alumina powder.

Key Words: Copolymer, aqueous alumina, electrosteric stabilization, adsorption, polymer molecular weight

A computational study of Cobalt Copper surface alloys and their stability

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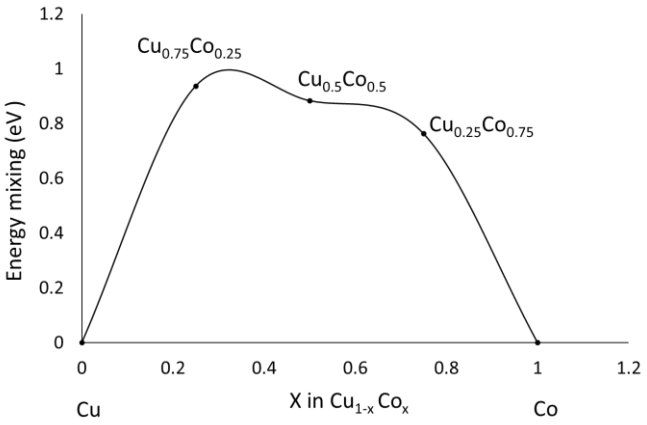

Profound interest has been laid on synthesis, characterization, and property evaluation of core/shell nanostructures due to their potential applications in various fields such as magnetism, optics, and catalysis. The phase stability of superstructures based on the Fcc lattice in the Co-Cu and Cu-Co (111) alloy surfaces are examined from the fully relativistic electronic density functional theory (DFT). The electron-ion interaction is described by the projector augmented-wave (PAW) method and the exchange-correlation effects are treated in the generalized gradient approximation (GGA). The surface expansion method is used to obtain effective atom-atom interactions on the Fcc lattice and is used also to guide a systematic ground state search for both alloy systems. The mixing energy analysis reveals a multitude of stabilized structures possibilities, especially at the Co-rich side. However, the segregation energy of different slabs revealed the existence of the remarkably stable Co based and Cu based alloys (Core/shell and single atom (SSA)) compared to the bulk alloys. The several models analyzed showed a difference of surface energy when inducing an alcohol on the surface. These results are critically compared with experimental data. It is shown that physicochemical properties of the two metals used, played a great role in adjusting the surface energy and controlling the hole NP stability.

Key words: Bimetallic CoCu, Surface energy, Density functional theory, dehydrogenation of alcohol

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Magnetic study of a new Cobalt (II) organic-inorganic hybrid material, $(C_6H_{16}N_2O)[CoCl_4]$

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In this work, a new cobalt hybrid compound $(C_6H_{16}N_2O)[CoCl_4]$was synthesized as single crystals by slow evaporation method at room temperature.

The single crystal X-ray diffraction study showed that the entitled compound crystallizes in the monoclinic system with the space group $P2_1/c$. Single-crystal X-ray diffraction analysis revealed that the atomic arrangement can be described as a succession of organic undulating chains parallel to [010] direction, integrating inorganic anions into columns running along a-axis. The different components are interconnected by N–H···O and N–H···Cl hydrogen bonds and weak Cl/Cl interactions which lead to a three-dimensional supramolecular network. Magnetic study of this compound included magnetic susceptibility measurements in the temperature range 2–300 K. The resulting $\chi_M T(T)$ curve showed that the complex has a paramagnetic behavior and magnetic inverse susceptibility χ^{-1} (T) plot fitted to the Curie-Weiss law suggested that our compound exhibits an antiferromagnetic exchange between the neighboring cobalt ions at low temperature.

Key words: hybrid compound, single crystal, magnetic susceptibility, Curie-Weiss law.

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A New 1-D polymeric chains of $(C_5H_6ClN_2)[CdCl_3H_2O]\cdot H_2O$ perovskite: Synthesis, Structure, Physico-Chemical Characteristics, Theoretical Calculations, and Biological Effects

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A novel 1D polymeric chains material $(C_5H_6ClN_2)[CdCl_3H_2O]\cdot H_2O$ perovskite was successfully synthesized with the use slow evaporation process. According to the single-crystal X-ray diffraction, the structure was deduced to crystallize in the monoclinic system (space group $P2_1/n$, no 14), with the cell parameters a = 17.8596 (9) Å, b = 7.5766 (2) Å, c = 18.2245 (9) Å, and β = 95.068 (4)°. The crystal packing is composed of infinite polymeric chains of $[CdCl_3H_2O]_n^{n-}$, that form with the organic cations layers parallel to the (10-1) plane and are held together by multiple H-bonds and Van der Waals interactions. The supramolecular assembly was also explored by the Hirshfeld surface study. The IR spectroscopic investigations were described to confirm the organic group's existence and define the corresponding vibration modes. The optical study was also used to show the semiconducting behaviour of this compound, which showed relatively low gap energy 2.8 eV, promising for diverse applications especially in tandem solar cells. The Arrhenius relation may be used to explain the conductivity of the material. In addition, the graphs of Z' and Z'' versus frequency were a perfect match to an equivalent circuit model, which was represented as a resistance linked in series with two parallel circuits (R//CPE). The chemical properties of the studied metal complex were investigated, and the properties of nonlinear optical effects (NLO) were also calculated. The molecular docking approach was utilized to determine the studied compound's interactions with breast, lung, liver, and colon cancer proteins, which were then examined in detail with PLIP analysis. In contrast, the Swiss-ADME analysis was performed to examine its pharmacological properties. Pathogenic microorganisms like *Klebsiella pneumoniae* and *Staphylococcus aureus* were also used to test how well the cadmium complex and antibiotics work together.

Key words: 1-D polymeric chains, Gap energy, DFT, Molecular docking, Swiss-ADME, Complex impedance spectroscopy, Antibacterial effect.

Sulfur-doped carbon nitride decorated with polypyrrole-coated N-doped titanium oxide for efficient remediation of dyes polluted water

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Innovative approaches, notably, adsorption and photocatalytic degradation, have emerged as promising technologies for addressing water contamination caused by both organic and inorganic pollutants [1]. These methods have proven effective in degrading persistent organic pollutants, such as dyes, known for their chemical stability and resistance to natural biodegradation in water. To this end, a novel nanocomposite was developed, consisting of sulfur-doped carbon nitride decorated with polypyrrole-coated N-doped titanium dioxide, aimed at synergistically adsorbing and photodegrading dyes, specifically Congo red and methylene blue. The physicochemical attributes were examined using various characterization techniques, including SEM and TEM microscopy, Raman, and XRD spectroscopy. Results from these analyses indicated that the chemical properties of the composite material, combining adsorption and photocatalysis, were notably influenced by the ratio of nitrogen-doped titanium dioxide and the proportion of adsorbent to photocatalyst. The adsorption and the photocatalytic studies revealed that the prepared nanocomposite exhibited significant adsorption and degradation efficiency, reaching up to 99.7% for both Congo red and methylene blue after 90 minutes.

Keywords: water pollution, photocatalysis, adsorption, dyes, nanocomposites.

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Novel ZnO/Ag heterostructures prepared from Ag^+-doped layered zinc hydroxides as highly active photocatalysts for the degradation of dyes and Ciprofloxacin

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The design and the synthesis of highly active nanohybrid photocatalysts for environmental remediation is a topical issue in the context of sustainable development. The hybridization of a semiconductor with noble metal nanoparticles (NPs) has been demonstrated to be a versatile strategy to restrict the recombination of photogenerated electron-hole pairs and thus increase the photocatalytic activity. However, the uniform association of nanosized metal particles with ZnO NPs remains a challenge. Herein, a novel synthesis of ZnO NPs hybridized with Ag(0) NPs is presented. Ag^+-doped layered zinc hydroxides (LZHs) were prepared in aqueous solution in the presence of triethanolamine and subsequently Ag^+ ions were photoreduced into metallic Ag NPs embedded into LZHs. The LZHs not only promote the dispersion of Ag NPs but also limit their growth. The Ag(0)-doped LZHs obtained after hydrothermal treatment was finally transformed into ZnO/Ag nanohybrids by a mild thermal treatment at 300°C for 5 min, which allows high interface coupling between ZnO and Ag NPs. ZnO associated with 3 mol% Ag exhibits the highest photocatalytic activity for the degradation of dyes (Rhodamine B and Remazol Brillant Blue R) and of the Ciprofloxacin antibiotic. The high photocatalytic performance of the ZnO/Ag(3) nanohybrid originates from the charge transfer in the ZnO/Ag nanohybrid and from the enhanced harvesting of visible light. The ZnO/Ag(3) photocatalyst also exhibits a high practical stability, indicating its great potential for real photocatalytic applications.

Keywords: ZnO, Ag, nanohybrid, charge transfer, photocatalyst, degradation

Structural, physicochemical characterization and antimicrobial activities of a tris(8-quinolinolato-κ^2*N*,*O*)cobalt(III) methanol solvate

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8-hydroxyquinoline, a quinoline derivative, enjoys a privileged status in medicinal chemistry, underlining the considerable importance of this class of compounds [1].
The crystal structure of the compound revealed a monoclinic system with space group *P*21/*n*. The asymmetric unit, shown in the **Fig. 1,** contain three deprotonated 8-hydroxyquinoline ligands, displayed a distorted octahedral geometry. Interestingly, the complex was found to crystallize alongside a methanol molecule, although it was not part of the cobalt coordination sphere. Structural cohesion primarily arose from π-π interactions between neighbouring quinoline rings and intermolecular hydrogen bonds connecting the cobalt complex units and uncoordinated methanol molecules.

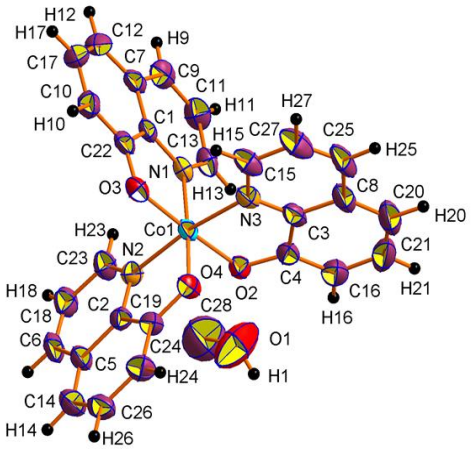

Fig.1 Asymmetric unit of compound $[Co(C_9H_6NO)_3].(CH_3OH)$

Notably, the compound demonstrated a significant antibacterial activity against *K pneumoniae* and *E coli*, and exhibited superior antifungal effects against *Candida* in comparison to the positive standard, owing to its anti-biofilm and anti-virulence action.

Key words: XRD, Band gap Energy, Hirshfeld surface analysis, Antibacterial and antifungal activities

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Development of Method for Quantifying Potassium Bromate in Bread Improver Additives

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Bread has long been recognized as a staple food that contributes significantly to the daily intake of essential nutrients in the human diet. The gluten present in wheat flour plays a key role in shaping the consistency of bread dough and its ability to trap gases generated during the fermentation process. To improve the quality of bread, the use of improver additives is often used in the baking industry. This practice arises from the ability of these agents to improve the handling properties of dough and improve the quality of fresh bread through the formation of disulfide bonds via the hydrogen sulfide groups inherent in protein chains. A wide variety of additives with different chemical structures are employed. The main class of additives used in baking is potassium bromate, which serves as an oxidizing agent and is considered one of the best and most cost-effective dough improvers in the baking industry. Due to its positive effects, it plays a significant role in the bread-making process. However, numerous reports have highlighted its negative impact on human health. Consequently, various techniques have been developed to determine the concentration of potassium bromate in bread. Therefore, the establishment of optimal methods and procedures for the rapid and accurate determination of potassium bromate content in bread remains of considerable commercial interest. NMR spectroscopy is currently a powerful tool for the qualitative and quantitative analysis of molecules of all types and sizes. This study begins by presenting the NMR profiles of commercially available improvers spiked with KBr to describe and compare their composition. These NMR profiles of commercial improvers could potentially be utilized for authentication purposes in the future. Subsequently, a rapid, reliable, and non-destructive method for quantifying KBr using 1D ^{1}H-NMR spectroscopy was developed and validated. The limits of detection (LOD) and quantification (LOQ) were found to be 0.05 and 0.15 mg/mL, respectively.

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Sol-gel synthesis of hollow TiO_2 microspheres with high photocatalytic activity

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Titanium dioxide is a photocatalyst widely used in wastewater treatment to combat the problem of pollution because of their low cost, high photosensitivity, non-toxicity and environmentally freindly nature [1]. With a wide band gap of around 3-3,2eV, TiO_2 has been extensively used in photocatalysis [2]. When TiO_2 is irradiated with UV light, electrons are excited from the valence band to the conduction band and electron–hole pairs are created. These electron–hole pairs activate the surrounding chemical species, and then promote the chemical reactions.

In this work the titanium oxide was prepared by sol-gel root. The synthesized product was caracterized by various techniques sach as X-ray diffraction, Raman spectroscopie and scanning electron microscopy. X-ray diffraction shows that the crystalline phase of the product is anatase. It also shows that the size of the particles is nanometric according to Debey-Scherrer equation. Raman spectroscopy confirms the X-ray diffraction results. With scanning electron microscopy, we see that the product is formed by hollow microspheres.

The photocatalytic activities of the photocatalysts are evaluated by the photodegradation of methylene blue under UV light irradiation.

Key words: sol-gel, titanium dioxide, photocatalyst, Debey-Scherrer, methylene blue

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Green synthesis, characterization and evaluation of antimicrobial behavior of magnetite nanoparticle

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Nanoparticles have great potential in various areas such as medicine, cancer therapy and diagnostics, biosensing, and material science. Iron oxide nanoparticles have demonstrated a promising effect in various biomedical applications. In particular, magnetite (Fe_3O_4) nanoparticles are extensively used for numerous bioapplications due to their biocompatibility, high saturation magnetization, chemical stability, large surface area, and easy functionalization. In this context,magnetite (Fe_3O_4) nanoparticles were successfully synthesized by a simple, rapid, and eco-friendly green method. The synthesized Fe_3O_4-NPs were characterized with X-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), Fourier transform infrared (FT-IR), and transmission electron microscopy (TEM) techniques. The X-ray diffraction planes (220), (311), (400), (422), (511), (440), and (533) were corresponding to the standard Fe_3O_4 patterns, which showed the high purity and crystallinity of Fe_3O_4-NPs had been synthesized. Based on FT-IR analysis, two characteristic absorption peaks were observed at 556 and 423 cm^{-1}, which proved the existence of Fe_3O_4 in the prepared nanoparticles. TEM image displayed the synthesized Fe_3O_4-NPs were mostly in spherical shape. The title compound gave strong antibacterial potential against gram positive and negative bacteria, it was able to affect growth and virulence factor of bacterial and fungal species.

KEYWORDS: *Fe_3O_4-NPs, Green synthesis, antioxidant; antimicrobial*

Experimental and Computational Survey of a Novel Cadmate Complex $(C_6H_{14}N)_2[CdCl_4]$ with Neurological Disease Inhibition Potential

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A novel Cd(II) complex, $(C_6H_{14}N)_2[CdCl_4]$, was successfully synthesized using the slow solvent evaporation method. Single crystal X-ray diffraction analysis revealed the centrosymmetrical nature of this compound, which crystallizes within the triclinic system, specifically in the space group $P\bar{1}$. The material's bulk phase purity and homogeneity were confirmed through powder X-ray diffraction analysis. The atomic arrangement of the title structure consists of isolated tetrahedral entities connected to the organic groups through weak hydrogen bonds (N–H…Cl and C–H…Cl), forming a three-dimensional network. Solid-state interactions were further studied through Hirshfeld surface analyses, along with 2D fingerprint plots. Computational results, obtained using the B3LYP method with 6-311++G(d,p)+LANL2DZ mixed basis set, demonstrated consistent geometrical, vibrational, and electronic properties to the experimental data. The frontier molecular orbital analyses and predicted molecular electrostatic potential map were also studied to illustrate the charge transfer phenomena within the structure. Non-covalent interactions were explored in depth through AIM and RDG analyses. To assess thermal stability, a comprehensive TG–DSC analysis was conducted. Furthermore, the inhibition activity of the studied compound was investigated *in-silico* via molecular docking studies targeting iNOS enzymes. These findings could pave the way for developing and testing innovative therapeutic interventions.

Key words: Cd(II) complex, DFT calculation, AIM-RDG, Thermal analysis, Molecular docking.

One-step synthesis of nanoparticle acid modified bimetallic cerium-zirconium oxide for fast fluoride removal from drinking water: Characterization and adsorption properties

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Removal fluoride from drinking water is still one of the most extreme environmental challenges facing humanity **[1]**. In the present investigation, a novel sulfated bimetallic oxide SO_4^{2-}-ZrO_2-CeO_2 (XSZC) xerogel adsorbent was prepared in one step by using the sol–gel method and developed for fluoride removal from drinking water. The nanoparticle XSZC material was characterized by BET, SEM, EDX, TEM, XRD and FTIR spectroscopy. Experimental conditions such as adsorbent dose, contact time, initial fluoride concentration and pH were optimized. The solid XZCS exhibits a high surface area (S_{BET} =255 m^2/g) and a large porosity (V_P = 0.30). The high surface area and rapid extraction kinetics of the SO_4^{2-}-ZrO_2-CeO_2 solid (contact time at equilibrium < 1min) makes this material among the top adsorbents currently known in fluoride removal. Furthermore, the result showed that XSZC has a high fluoride removal rate of approximately100% in the wide pH range (2-8) with a low adsorbent dose (30mg). The Freundlich isotherm model can better describe the behavior of SO_4^{2-}-ZrO_2-CeO_2 fluoride adsorption. The adsorption kinetic process follows the pseudo-second-order kinetic model. FTIR spectroscopy proves the important role of both superficial hydroxyl groups and the sulfate anion in the defluorination process. The nanoparticle SO_4^{2-}-ZrO_2-CeO_2 adsorbent showed a high potential for the removal of fluoride from real drinking water.

Key words: Fluoride adsorption, Cerium- zirconium oxide, Nanoparticle, Drinking water

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Novel Cobalt Hybrid Material with Ionic Organic Cation: Crystal Structure, Electrical Conductivity, Photoluminescence and Magnetic Properties Studies*

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Hybrid materials have become increasingly important in the materials science field as they offer unique properties that cannot be found with traditional materials. A hybrid material is a combination of two or more distinct materials that, when combined, create a novel material with enhanced or altered properties of the original materials. These properties can include magnetic, electrical, chemical, thermal, and optical properties. In this study, we successfully synthesized a new hybrid compound through a slow evaporation process at room temperature. It was thoroughly characterized using single X-ray diffraction SXRD, photoluminescence (PL) spectroscopy, thermal analysis (DSC, TG/DTA), and photoluminescence (PL) spectroscopy, magnetic analysis, and proton conductivity study.

The SXRD analysis at room temperature of the new hybrid compound crystallizes in the triclinic *P-1* space group and formulated as $[(C_2H_3N_4)_2CoCl_3\cdot(HCl)(H_2O)]$. The structural integrity of these compounds is maintained by an extensive network of hydrogen bonds, π-π interaction, and electronegative interaction. PL spectrum was analysed and indicated that this material exhibits a green and yellowish photoluminescence and showcase of charge transfer phenomenon. The magnetic measurements perform on the title compound show a paramagnetic behaviour under the temperature range analysed. In addition, it exhibits a moderate proton conductivity, reaching a value of $5\cdot10^{-4}$ S cm^{-1} at 428 K in anhydrous conditions. Finally, the thermal analysis confirm that this anhydrous compound shows a thermal stability up to 450 K then it decays in four successive steps losing 83.39% of total weight.

Key words: SXRD, DSC, TG/DTA, magnetic, proton conductivity, PL.

Degradation of amoxicillin by anodic oxidation

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Amoxicillin is one of the most used antibiotics worldwide for bacterial infection treatment caused by positive and negative gram. It is a-amino-substituted β -lactam antibiotic belonging to the penicillin class. The amoxicillin was selected as target pollutant and the oxidative degradation was ensured by hydroxyl radicals generated. Electrochemical degradation of amoxicillin has been extensively studied in an undivided electrolytic cell. The removal of amoxicillin was studied as a function of pH, effect of current density and effect of electrolytes support. Mass spectrometry was employed to identify major transformation by-products of AMX electrochemical degradation.

Keywords: Amoxicillin, degradation

Structure, physico-chemical characterizations and Hirshfeld surface analysis of $[C_7ON_2H_{18}]_3V_{10}O_{28}\cdot 2H_2O$ compound

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A new decavanadate compound, tri[2-[2-(dimethylamino) ethyl-methylaminium]ethanol] decavanadate dehydrate, was synthesized by slow evaporation, the formula unit is composed by one decavanadate cluster, three $[C_7ON_2H_{18}]^{2+}$ organic cations and two water molecules. Different characterization techniques are used such as: crystal X-ray diffraction, SEM-EDX analysis and thermal analysis. The X-ray structure determination revealed that the compound crystallizes in the triclinic system, space group P-1 with the cell parameters: a= 10.815(9) Å, α= 112.97(3)°, b=11.624(4) Å, β= 111.73(7)°, c= 11.840(5) Å, γ= 96.86(6)° and **V=1195.8(6).** The cohesion of the structure is ensured by hydrogen bonds of the type O-H...O, N-H...O and van der Waals interactions. The study of the Hirshfeld surface of the decavanadate compound shows us that it is dominated by O…H/H…O (56.7%) and H…H (30.2%) type contacts.

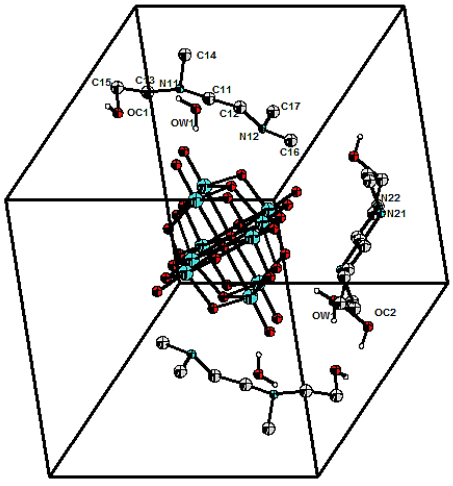

Figure 1. Formula unit of $[C_7ON_2H_{18}]_3V_{10}O_{28}\cdot 2H_2O$ compound

Keywords: Decavanadate, X-ray diffraction, Hirshfeld surface, SEM-EDX

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Optical properties of SiNWs by the deposition of snowball-like V_2O_5 nanoparticles

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In this work, the morphological and optical properties of vanadium pentoxide (V_2O_5) nanoparticles deposited on silicon nanowires (SiNWs) have been investigated. SiNWs are obtained by metal-assisted chemical etching (MACE) method. The deposition of vanadium pentoxide on SiNWs layer was performed by vacuum thermal evaporation system for different durations. Scanning electronic microscope (SEM) images show the formation of snowball-like V_2O_5 nanoparticles on the SiNWs surface. A large condensation of V_2O_5 elements was observed by increasing the evaporation time. The changes in bonds and chemical composition at the surface of the SiNWs-V_2O_5 nanocomposites were examined by Raman and Fourier transform infrared (FTIR) spectroscopies. The X-ray Diffraction (XRD) technique revealed the presence of orthorhombic structure of V_2O_5 layer with good crystallinity. The SiNWs-V_2O_5 composites show strong visible PL due to the contribution of the radiative band edge transitions of vanadium pentoxide. The emission of V_2O_5 layer is in the same energy range as that of SiNWs thus leading to a large increase in PL intensity. Optical band gap (Eog) was determined from UV–Vis-IR spectroscopy. The presence of vanadium pentoxide on the SiNWs surface causes an increase in the value of E_{og} from 1.851 to 2.075 eV. This increase was explained by Burstein-Moss effect.

Synthesis, Spectral, crystal structures, DFT and thermal investigations on Fe^{3+} complexes of favipiravir ligand

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The appearance of the COVID- 19 virus caused a crucial widespread pandemic with shocking social and economic challenges for the global society worldwide. Favipiravir, chemically known as 6-fluoro-3-hydroxypyrazine-2-carboxamide, is a drug that has shown promising results in treating diseases. In the solid state, Favipiravir lies completely flat and is stabilized by an intramolecular hydrogen bond (O–H---O), forming a six-membered pseudo-aromatic ring. In solution, it exhibits a highly complex polyfunctional tautomeric system. The rotation of the amide and hydroxyl groups introduces additional isomeric possibilities for each tautomer. The corresponding relative energies of the structures show that the enol tautomer is significantly more stable than the keto one in most of the aprotic organic solvents independently of the solvent's polarity. In the presence of water or protic solvent like methanol and ethanol, a keto form appears to be favored due to the specific solute–solvent interactions.

Novel metal chelates were synthesized by reacting Fe (III) ions with the Favipiravir ligand in a methanolic solution of the metal salt. Upon the addition of iron-metal ions, simultaneous deprotonation and complexation occurred, resulting in the formation of 2:1 ligand-to-metal complexes. The synthetic process was thoroughly detailed, and the prepared compounds were analyzed using various analytical and spectroscopic techniques, including IR, 1H NMR, UV–Vis, X-ray (RX), and TGA/TDA, to elucidate their structures. Furthermore, both the ligand and its metal complexes were geometrically optimized using Gaussian 09 based on DFT theory.

Key words: Favipiravir, Metal chelates synthesis, Characterization, DFT.

Dimethyl ether production from syngas over composite Cu-ZnO (Al)-Xerogel ZrO_2/SO_4^{2-} catalysts

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The growing energy demand, coupled with the depletion of fossil fuel resources, along with the adverse effects of greenhouse gas emissions on climate change, have boosted investigations of alternative renewable resources that are readily available, sustainable and eco-friendly [1]. Among the greenhouse gases, a great deal of attention has been paid to carbon dioxide (CO_2) in recent years. One of the CO_2 recovery products is dimethyl ether (DME). Its non-carcinogenicity, low toxicity, non-corrosive, easy storage, and transportation, its similarity to liquefied petroleum gas (LPG) in terms of its physical properties, all these properties make it an ideal substitute to traditional fuels [2]. Nowadays, DME is produced through a one-step process using bifunctional catalysts in a single reactor. These catalysts facilitate both the hydrogenation of methanol from syngas over metallic function and the dehydration of methanol to DME over acid function.

The catalytic performance of combined Cu-ZnO (Al) catalyst (CZA) and xerogel sulfated zirconia (acid catalyst) has been investigated in the direct synthesis of DME from syngas. CZA catalyst was synthesized using co-precipitation method with optimized composition (Cu/Zn/Al = 68/29/3). The acid catalyst was prepared via sol-gel “one put” method, then calcined at 300°C and 560°C. The mixed catalysts containing CZA and acid catalyst were prepared by physical mixing. Obtained solids were characterized with various techniques such as N_2 adsorption-desorption, ATR-FTIR spectroscopy, XRD, H_2-TPR and NH_3-TPD-MS. The catalytic properties show that the CZA catalyst mixed with the acid catalyst before calcination is more active and selective for the production of DME from the synthesis gas under the same reaction conditions (250°C, 30 bar) than if it is mixed with the acid catalyst calcined at 300°C and 560°C. This result is closely related to the appropriate metallic surface, structure and more developed acidity of catalyst.

Key words: DME from syngas, xerogel sulfated zirconia, CZA, Acidity.

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Valorisation and Treatment by Ultrafiltration of effluents from the fishing industry

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The seafood processing industry consumes water and generates large quantities of waste, including solid discharges as well as wastewater that is discharged as effluent. Process water is generally rich in pollutant load (chemical oxygen demand (COD)), organic matter and has high turbidity. Therefore, the direct discharge of these waste streams has the potential to degrade receiving aquatic environments through localized dissolved oxygen depletion, eutrophication and aquatic toxicity. At the same time, it has been demonstrated that these effluents constitute a deposit of biomolecules of interest, in particular proteins. These effluents are therefore widely available raw materials and for which many uses are possible both in animal and human food.

Membrane processes, thanks to their intrinsic properties, must be considered as a valid alternative for the recovery of these effluents according to the principles of a sustainable circular economy. This work focuses on the treatment of washing water from a shrimp packaging line in an industrial facility located in the region of Sfax, Tunisia, by ultrafiltration (UF) at the laboratory scale. Filtration experiments were performed using flat-sheet organic membrane module. The ultrafiltration membranes used were polyethersulfone (PES) with a molecular weight cut-off MWCO) of 50, 10, and 5 kDa. All the experiments were carried out at an ambient temperature of 20° C and at a pressure of 2 bar. The protein concentration of this shrimp washing water consists of an ultrafiltration-diafiltration step. The procedure was as follows: an initial phase of ultrafiltration (UF) with total recycling of the retentate, immediately followed by diafiltration (DF). The unfiltered washing waters, the permeate and the UF concentrate were analyzed for pH, conductivity, turbidity, dry matter, ash content and protein content. The chemical oxygen demand (COD) was determined in the original water and in the permeate. UF treatment with 50 and 10 kDa membranes significantly improves the quality of the effluent. In addition, better results were obtained for the physico-chemical parameters. COD was significantly reduced (approximately 73 and 92% respectively). However, the residual COD in the permeate was always above the discharge limit imposed by the standards (200 mg. L^{-1}). More promising results were obtained with the 5 kDa membrane with in particular a protein recovery percentage of 91%. A significant reduction in the COD with a rejection rate of 96%, respond thoroughly to the enforced norms. This result indicates that ultrafiltration has been used successfully to concentrate proteins and reduce COD in the washing water discharged from the shrimp processing plant. In conclusion, ultrafiltration proves to be viable both in the recovery of valuable compounds such as proteins and in the depollution of waste, thus contributing to the sustainability of the seafood processing sector.

Keywords: ultrafiltration, washing water, proteins, depollution

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Rare-earth doped fluoride ZLAG and ZLBA glasses for solar energy conversion

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Rare-earth (RE) ions as luminescence centers incorporated into different hosts have attracted more attention due to their potential technological applications in many fields as solid lasers **[1]**, planar waveguides **[2]** and up- or down-convertors in photovoltaic **[3]**.

Solar cell conversion efficiency is limited to 30% because only the photons with energy close to the semiconductor's bandgap energy (that is a wavelength lower than 1100 nm) can be profitably absorbed by the solar cell **[4]**. Recently, down-conversion (DC) mechanism can be exploited to convert one visible photon into one or two near infrared (NIR) photons where silicon (Si) solar cells are efficient. The choice of the matrix is important to obtain a good efficiency.

Single-doped Tm^{3+} and co-doped Tm^{3+}/Yb^{3+} fluoride glasses based on ZLAG and ZBLA been prepared by the conventional melting-casting method.

We used several techniques for the characterizations of the samples. The absorption spectra were obtained from a Perkin Elmer Lambda 1050. Photoluminescence (PL) and decay time measurements were performed in the visible and NIR using a spectrofluorimeter with a xenon lamp as excitation source. All the measurements were carried out at room temperature.

Single-doped Tm^{3+} and co-doped Tm^{3+}/Yb^{3+} fluorozirconate glasses have been successfully synthesized and tested as down-convertor encapsulation glasses for Si-solar cells. Spectral modification from visible region to NIR region was realized via cooperative energy transfer from Tm^{3+} to Yb^{3+} which proved by photoluminescence measurments.

Key words: Rare earth, solar cells, fluorozirconate glasses, photoluminescence.

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Synthesis, Crystal structure, Thermal, Spectroscopy, Optical and Photoluminescence Properties of a novel hybrid compound bis (4-fluorobenzylammonuim) tetrachloridozincate

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A novel organic-inorganic hybrid material $[C_7H_9NF]_2ZnCl_4$ was obtained by slow evaporation at room temperature and characterized by single crystal X-ray diffraction. The compound has monoclinic space group $P2_1/n$ with the following cell parameters: $a = 15.1956(10)$ Å, $b = 7.2108(3)$ Å, c = 36.103(2) Å, $\beta = 93.1(6)°$, $V = 3950.1$ Å^3 and $Z = 8$. The crystal structure consists of tetrahedral $[ZnCl_4]^{2-}$ anions and 4-fluorobenzylammonuim $[C_7H_9NF]^+$ cations connected by hydrogen bonding N–H···Cl, C–H···Cl, π-π, and van der Waals interactions, which ensure the stability of the crystal packing, forming layers laying approximately within the (101) planes. Powder XRD demonstrates the remarkable phase purity of both crystals. Infrared spectroscopy confirms the presence of the organic moiety in the structure, and the material exhibits thermal stability up to 180°C. Hirshfeld surface analysis reveals the significance of hydrogen bonds and electrostatic interactions in the material cohesion, while 2D fingerprint plots indicate the contributions of the H...Cl and H…H intermolecular interactions. The material also displays diffuse absorption, indicating the existence of optical direct allowed transition mechanisms with the band gap energy equal to 4.33 eV. Its photoluminescence spectrum extends over all visible band when it is excited by a Ultra-violet radiation owing these properties; the compound is promising for optical devices.

Keywords: Organic-inorganic hybrid material; Single crystal X-ray diffraction; Crystal structure; Hirshfeld surface, TGA/DTA, Powder XRD, Vibrational study, Optical absorption, Photoluminescence.

Development and validation of a method for analyzing calcium carbonate in the raw state and after grinding by X-ray diffraction

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Aims of the work:
As part of our work, we are interested in developing and validating a method of analysis by X-ray diffraction - XRD and laser granulometry according to the ISO / IEC 17025 standard and in the reduction of the particle size of the calcium carbonate by the grinding input.
Methods:
To do this, a comparative study was carried out by optical microscopic techniques, DRX, DSC and FTIR were used to characterize the solid state of calcium carbonate before and after grinding under different conditions.
Laser granulometry is an analysis method that allows you to determine the size particles (0.02 to 2000 µm) suspended in liquid or air based on the principle of laser diffraction by the theory of Fraunhofer and Mie.
Results:
The results found allow us to carry out the reduction in the size of the calcium carbonate particles and we can characterize the microstructural and structural changes induced during the processes of reduction of the size of the particles of calcium carbonate.
Conclusion:
Calcium carbonate is a is a calcium salt with formula CaO_3. It has a role as an antacid, a food colouring, a food firming agent and a fertilizer. It is a calcium salt, a carbonate salt, a one-carbon compound and an inorganic calcium salt.. This calcium salt is practically insoluble in water. The particle size distribution of calcium carbonate affects their solubility as well as their rate of dissolution.We have developed a method analyzing calcium carbonate in the raw state and after grinding by X-ray diffraction.

Key words: Calcium carbonate, Development, Validation, Laser Granulometry, DRX, FTIR.

Growth, Single crystal investigations, Synthesis, Spectroscopic characterization, and Electrical and Biological studies of novel hexaisothiocyanato Chromate complex

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We successfully synthesized 3D supramolecular structure of 2-Amino-6-methyl piridinium hexaisothiocyanatochromate (III) complex, $(C_6H_9N_2)_3$ $[Cr(SCN)_6].H_2O$.The desired complex was confirmed and we obtain the triclinic crystallinity having $P\bar{1}$ space group of as-grown crystals has been revealed by single X-ray diffraction analysis (XRD) **[1]**. The novel complex was characterized by various techniques, such as FTIR analysis, solid state UV-Visible and fluorescence to investigate the optical property **[2],** add to the biological behavior by the evaluation of anti-free radical activity by trapping free radical (DPPH) **[3]** and impedance complex analysis to investigate mainly its interesting properties as well **[4]**.

Key words: Transition metal, Chrome (III), Crystal structure, Optical, Hirshfeld surface, Antioxidant property, Electric behavior.

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Adsorption of Acetaminophen from aqueous solution using Chitosan Beads extracted from Shrimp Shells

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In this work, chitosan was synthesized from shrimp shell waste (Parapenaeus longirostris) obtained from the local market of eastern Algeria (Annaba), a chemical process was followed containing 4 successive steps (demineralization, deproteinization, decolorization, deacetylation). The chitosan beads were synthesized via a physical modification of the extracted chitosan and characterized using FTIR, XRD techniques. The degree of deacetylation (DD%) is calculated from the FTIR data.

The chitosan beads were utilized for Acetaminophen (paracetamol) removal from synthetic water. The batch adsorption process was optimized, and the impact of Contact time and the adsorbent dosage were analyzed. the kinetics and equilibrium analysis were done, the results showed that the adsorption kinetics agrees with the pseudo second-order.

Key words: Acetaminophen, Chitosan synthesize, Chitosan beads, Adsorption.

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Development of a disk ceramic membrane based on Tunisian clay: Application to treatment of wastewaters

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Research in the field of ceramic membranes for wastewater treatment is growing rapidly due to their high chemical, thermal and mechanical stability, high separation efficiency and long service lives.

The aim of this work is the preparation of a low-cost membrane from Tunisian clay and phosphate sludge in order to be used in a filtration process. The mineralogy of materials is obtained by X-ray Diffraction (XRD), the geochemistry by X-ray fluorescence (XRF), the thermal behavior is obtained by Differential Thermal Analysis (DTA) and Thermogravimetric analysis (TGA).

The chemical analysis and mineralogy of clay materials show a majority of silicic oxides SiO2 (36.59%) and aluminum oxides Al2O3 (11.29%), smectites (55%), kaolinite (22%), quartz (1%), gypsum (3%), calcite (15%) and dolomite (4%). While the phosphate sludge is essentially consists mainly of fluoroapatite (48%), calcite (32%) and clay.

After characterizing the clay and phosphate sludge, these were mixed with well-determined quantities, pressed and sintered at 1100 °C for 2 h to obtain flat ceramic membranes of 44 mm in diameter and 3-5 mm in thickness.

Different characterizations were carried out to determine the porosity (water absorption, observation under a scanning electron microscope), the mechanical resistance of these membranes; the samples have good porosity (from 1 to 20 µm), high compressive strength.

These membranes show good efficiency in removing pollutants from wastewater. The integration of phosphate sludge improves the properties of ceramic membranes and the management of large quantities of phosphate waste and thus minimizes their harmful impact on the environment.

Key words: Ceramic membrane, clay, filtration test, phosphate sludge.

Chitosan-modified molybdenum disulfide decorated with silver-doped zinc oxide for synergetic adsorption and photodegradation of dyes

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The increased importance of the impact of organic dyes on the environment and human health has emerged as a crucial concern, primarily owing to their adverse effects on human well-being and their capacity to disturb the ecosystem. Nevertheless, the effort to develop highly effective materials for the absorption and degradation of organic dyes poses a notable challenge in practical implementation within the academic domain. From this standpoint, a novel approach involved the development of a chitosan-modified molybdenum disulfide modified with silver-doped zinc oxide nanoparticles to purify dye-contaminated wastewater. The physicochemical features of the developed nanocomposite were evaluated through various characterization techniques, encompassing SEM and TEM microscopies, Raman, and XRD spectroscopies. Adsorption and photocatalytic degradation investigations were conducted on hazardous textile dyes, namely Methyl Orange (MO) and Congo Red (CR). The findings revealed that the prepared nanocomposite exhibited a maximum degradation efficiency of up to 99.1% for MO after 25 minutes and 97.6% for CR after 90 minutes.

Keywords: water pollution, photocatalysis, adsorption, dyes, nanocomposites.

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IR and Raman spectra of Zinc Sulfide (ZnS)
A Quantum Mechanical simulation of its Frequencies and Intensities

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Through first-principles calculations, we investigate structural stability, vibrational and linear and nonlinear optical properties of the zinc sulfide (ZnS) in different periodic forms ranging from the 3D bulk to the 2D hexagonal monolayer and their corresponding 1D zigzag single-walled nanotubes. First, the electronic wave function on the ground state was constructed using linear combinations of Gaussian-type functions at the DFT/B3LYP level. Then, the Raman and IR spectrum is computed using a Coupled-Perturbed-Hartree-Fock/Kohn-Sham (CPHF/KS) approach.Cohesive, relaxation, rolling energies, elastic and piezoelectric constants, electronic and nuclear contributions to the polarizability tensor, and nonlinear first and second-order hyperpolarizability tensor components are reported. Our study shows that 3D and 2D forms are stable and show semiconducting behavior, good piezoelectric responses, and fascinating linear and nonlinear optical properties. For 1D single-walled nanotubes, dynamic stability is observed only for the smallest (6,0) nanotubes. For n > 6, imaginary mode frequencies in the simulated IR and Raman spectra indicate dynamic instability. Scanning mode procedure along the largest imaginary vibrational mode is applied in order to determine the stable structures of the largest (14,0), (18,0), and (22,0) ZnS nanotubes. Therefore, it is worth mentioning that no imaginary phonon frequencies are detected in their vibrational spectra. Their potential energy surface contains two minima between a saddle point corresponding to a slightly distorted nanotube structure. Our study proves that the zinc sulfide nanostructures possess diverse physical properties that are useful for potential applications in nanoelectronics and nanodevices.

Key words: DFT, Vibrational modes,

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Synthesis, molecular structure, Vibrational studies, Thermal behavior and Optical properties of Supramolecular Hybrid perchlorate

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A hybrid material 4-aminopiridinium perchlorate salt $(C_{10}H_{13}N_4)ClO_4$ was synthesized at room temperature by slow evaporation and characterized by single crystal X-ray, spectroscopic (FT-IR, Raman and UV-Visible), thermal studies (TGA and DSC). The crystallographic data given from single crystal X-Ray showed that the compound adopts the monoclinic system, space group P2 1 /n with the following parameters a = 10.8317(8) Å, b = 9.0529(5) Å, c = 13.7032(9) Å, β = 99.243(3) °, Z = 4 and V = 1326.27(15) Å 3. The stability of the supramolecular structure was ensured by hydrogen bonding contacts N-H…O lengths that are ranging between 3.065 and 3.167 Å. According to Hirshfeld analysis results O...H interaction is the main intermolecular interactions contacts (46%). The thermal decomposition of the precursors studied by TGA and DSC analysis indicates that the compound presents a thermal stability up to 130°, then its degradation. Infrared and Raman spectra were recorded at room temperature, confirmed the existence of vibrational modes corresponding to organic and inorganic groups. In addition, the optical properties of the synthesized compound show UV-Visible absorption and interesting photoluminescence properties. Related HOMO-LUMO orbital energies were also highlighted using TDDFT calculations at B3LYP/6-31G(d,p) level of theory.

Antibacterial activity of the essential oil of *origanum glandulosum* on bacterial strains of hospital origin most implicated in nosocomial infections

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The fear of microbial contamination in hospitals is a current phenomenon. Indeed, nosocomial infections have become a major public health problem. Some bacterial species have adapted to antibiotics that are less sensitive to and develop multiple resistance. The objective of our research is to propose a solution to problems associated with bacterial resistance in hospitals, our interest is focused on the Origanum glandulosum, one of the most cited aromatic plants for its antimicrobial properties. The objective is to demonstrate the effectiveness of its essential oil that we will extract ourselves by pharmacognosy processes, and to compare it to previous studies. The originality of this work is the use of essential oils on multi-resistant bacteria, even highly resistant.

The extraction of the essential oil was performed by water steam distillation; the yield obtained from the aerial parts (1.78%) is interesting, its chromatographic profile revealed by TLC showed the presence of phenolic compounds thymol and carvacrol. The evaluation of the activity of the essential oil of *Origanum glandulosum* on bacterial strains of hospital origin, ATCC, MRB, and HRB, most implicated in nosocomial infections (Staphylococcus aureus ATCC 25923, Staphylococcus aureus ATCC 43300, Enterococcus faecalis ATCC 29212, Escherichia coli ATCC 25922, Pseudomonas aeruginosa ATCC 27853, Staphylococcus aureus resistant to meticillin, Enterococcus faecium, VA R and R TEC, Acinetobacter baumanii, IMP R and R CAZ, Klebsiella pneumonia carbapenemase-producing) by the method of aromatogramme and microatmosphere, shows that the antibacterial potency of this oil is very high, expressed by significant inhibition diameters on all strains except Pseudomonas aeruginosa, and low MICs and is characterized by a bactericidal action.

Keywords: Essential oil, nosocomial infections, *Origanum glandulosum*, MBR, HRB, antibacterial activity.

Constant Rate Thermal Analysis of Calcium Atorvastatin Trihydrate and the Influence of Grinding on its Thermal Stability, with an Exploration of Activation Energy

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The pathways of thermal dehydration reaction of both, calcium atorvastatin trihydrate (CAT) and grinded CAT, were investigated using Constant Rate Thermal Analysis (CRTA) technique under controlled residual water vapor pressure of 5 hPa using complementary analysis techniques, namely TG, DSC and XRD. The results show that CAT sample is a pure atorvastatin in its trihydrated form and that, under CRTA conditions, it dehydrates in three separated steps between 261 K and 393 K, each corresponds to the loss of one water molecule. On the other hand the grinded CAT dehydrates in one step. From the duration of the CRTA experiment and the X-ray diffraction technique we have showed that the grinding partially dehydrates CAT, to obtain calcium atorvastatin $1.5H_2O$, while decreasing its crystallinity. Also, examination by X-ray diffraction technique of the CRTA final products of both, CAT and grinded CAT, showed that the anhydrous phase of CAT is crystallized whereas the one of the grinded CAT is amorphous. The apparent activation energies corresponding to the dehydration steps of CAT and grinded CAT were experimentally measured by means of two CRTA curves realized at two different reaction rates without any hypothesis on the kinetic model of the reaction. They were found equal to 39 $kJ.mol^{-1}$ and 34 $kJ.mol^{-1}$ for CAT dehydration and 126 $kJ.mol^{-1}$ and 289 $kJ.mol^{-1}$ grinded CAT dehydration.

Keywords: CRTA; heterogeneous kinetic; calcium atorvastatin trihydrate; XRD; Activation energy

Pencil Graphite Electrocatalytic Sensors Modified by Pyrene-Reduced Graphene Oxide Decorated with Molybdenum Disulfide Nanoroses for Hydrazine and 4-Nitrophenol Detection in Real Water Samples

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A nanostructured platform, denoted as MoS2NRs/PCA-rGO/PGEs, has been innovatively engineered for the electrocatalytic detection of harmful pollutants-hydrazine (N2H4) and 4-nitrophenol which pose significant threats to the environment and human health [1]. The electrocatalytic system entails the modification of Pencil Graphite Electrodes (PGEs) through the application of pyrene carboxylic acid (PCA) functionalized Reduced Graphene Oxide (rGO), followed by the chronoamperometry electrodeposition of MoS2 nanoroses (NRs). A comprehensive characterization of the MoS2NRs/PCA-rGO/PGEs was conducted using various microscopic, spectroscopic, and electrochemical techniques, affirming the dense multilayer coating of PCArGO/PGEs by NRs. The sensing processes of N2H4 and 4-nitrophenol were monitored through Differential Pulse Voltammetry (DPV), revealing the superior electrochemical and electrocatalytic performance of MoS2NRs/PCA-rGO/PGEs compared to both unmodified PGEs and those exclusively modified by PCA-rGO. These nanoplatforms demonstrated remarkable sensitivity, selectivity, repeatability, reproducibility, and storage stability with low detection limits, exceeding the concentrations recommended by the U.S. EPA for drinking water. The efficacy of the nanoplatform in monitoring N2H4 and 4-nitrophenol levels in water environments was successfully validated.

Keywords: water pollution, electrocatalysis, sensing, electrodeposition, nanocomposites.

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Synthesis and crystal structure of hybrid compounds based on tin(IV) : Comparison of the fluorides with the chlorides.

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So-called 'zero-dimensional' hybrid perovskites are characterized by a structure formed by isolated inorganic octahedra (or bioctahedra) and an organic cation [1]. They are easy to prepare using simple techniques and they combine the properties of the various organic and inorganic components, i.e. the flexibility of the organic part, and the thermal stability and the rigidity of the inorganic part, in a single material, by cooperative effects, to obtain properties that are more than just the sum of the initial properties: an organic/inorganic 'synergy' is created [2]. For example, in these hybrid materials, the organic part can have non-linear optical properties. Most of the physical properties come from the inorganic part, such as the electronic transport properties and the optical photoluminescence properties [3, 4]. Antibacterial properties were also observed. The following tin-fluorine based compounds were prepared and investigated:

- Tris pyridiniumfluoro tris oxalato stannate(IV) monohydrate, $3(C_5H_6N)(C_2O_4)3SnF.\ H_2O$.
- Difluorotetrachlorostannate(IV) dipyridinium, $(C_{10}H_{10}N_2)SnF_2Cl_4\ .\ H_2O$.
- Bis 1.10–phenanthrolinium cis di fluoro bis oxalate stannate(IV) dehydrate, $2(C_{12}N_2H_9)(SnF_2(C_2O_4)_2\ .\ 2(H_2O)$.
- Bis(3-carboxyanilinium) hexachlorostannate(IV), $(C_7H_8NO_2)2SnCl_6$.

Key words: Hybrid compounds, fluorostanne(IV), X-rays diffraction.

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Structural study, spectroscopic characterization, thermal properties and evaluation of the antimicrobial behavior of a new Fer (III) organic-inorganic hybrid material: $(C_8H_{14}N_2)_4[(FeCl_6)(FeCl_4)]Cl_4$

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The organic-inorganic hybrid compound with the formula $(C_8H_{14}N_2)_4[(FeCl_6)(FeCl_4)]Cl_4$ was synthesized via slow evaporation at room temperature, and characterized using various techniques including X-ray powder diffraction (XRD), FT-IR, UV-Vis spectroscopies, and thermal analysis. The compound was found to crystallize in the tetragonal system, with $I4_{1/a}$ space group. In the crystal structure, the inorganic layers contain one octahedral $(FeCl_6)^{3-}$ ion, one tetrahedral $(FeCl_4)^{-}$, and four uncoordinated chlorine anions. The organic layers are made of four protonated m-Xylylenediamine $(C_8H_{14}N_2)^{2+}$. The structure is held together by N-H…Cl hydrogen bonds and Cl…Cl interactions. Powder XRD analysis confirms the purity of the crystalline phase, while UV-Vis spectroscopy indicates that the compound exhibits semi-conductor behavior. FTIR spectroscopy was performed to identify the functional groups present in the crystal structure. Thermal analysis was also carried out. Analysis of the Hirshfeld surface revealed that the H…Cl/Cl…H interactions dominate the structure (74%). The new Fe(III) complex gave strong antibacterial potential against S. aureus, E. coli, M. luteus, it was able to inhibit growth of Candida species and Trichophyton intergiditale and showing lysozyme activity.

Keywords: Organic-inorganic hybrid; XRD; thermal analysis; Hirshfeld surface analysis; antibacterial

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Synthesis of Ti_3AlC_2 Nanopowders by Mechanical Alloying for Energy Storage Application

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In this work, Ti_3AlC_2 nanopowders were prepared at room temperature through mechanical alloying (MA) from Ti, Al, and C elemental powders. MA process was carried out in a planetary ball mill under argon atmosphere. Structural and microstructural changes of the milled powders were investigated by X-ray diffraction (XRD), scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM/EDX), and transmission electron microscopy (TEM). XRD results showed that the desired Ti_3AlC_2 phase was obtained after 20 h of milling. SEM observations revealed that the powder milled for longer milling time was composed of agglomerated particles with near-spherical shape. TEM analysis of powder MA for 20 h confirmed that the Ti_3AlC_2 nanopowders with particle size of about 20 nm.

Key words: Ti_3AlC_2, Microstructure, Mechanical Alloying, Nanostructure

Development and characterization Polypyrrole/$NaxCoO_2$ for application as electrodes in energy storage systems

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The lamellar oxide "$NaxCoO_2$" is the most beneficial material for use as a positive electrode for sodium-ion accumulators, despite the success of sodium cobaltite, which is currently the most widely used. In addition, its structural modification that limits the insertion-disinsertion phenomenon motivated us to design and synthesize a new composite material «Polypyrrole/$NaxCoO_2$» whose capacity of oxide alone was tried to improve which is about 150 $mAhg^{-1}$, by the presence of a conductive polymer.

Great interest is given to conductive polymers which have found their applications in different industrial fields thanks to their typical stabilities, their simple and inexpensive syntheses, as well as its structure which provides a maximum degree of conjugation hence the ability to give high electrical conductivities.

Our work aims to improve the electrochemical performance of materials used as cathode in the sodium-ion battery, using a conductive polymer that serves to protect the spray electrode during electrochemical reactions. The lamellar oxide $NaxCoO_2$ was synthesized by the soil-gel method[1] using a complex agent. Polymerization was produced by oxidative polymerization of the monomer and ammonium persulphate in a HCl[2] solution. Polymerization was carried out by varying the amount of starting monomer in order to modify the thickness of the polymer layer on the oxide surface.

Various characterization techniques such as X-ray diffraction (DRX), thermogravimetric analysis (ATG), differential scanning calorimetry (DSC), Fourier transform spectroscopy (FTIR), UV-spectroscopyVisible and Raman spectroscopy and scanning electron microscopy (SEM). The analyses showed that all the materials developed have the same structure including the P6/3mmc space group. All materials also showed similar morphology and nanometric particles.

Keywords: conductive polymers, polymer/$NaxCoO_2$ composites, sodium-ion batteries.

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Silver nanoparticle-containing mesoporous silica-based systems for iodine entrapment and immobilization from gas phase

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Submicron-in-size silica particles with controllable morphology, particle size and mesoporosity, have been prepared under basic conditions making use of cationic alkyltrimethylammonium surfactants as porogens. Gaseous nitrogen adsorption, XRD and TEM experiments revealed quasi-spherical homodispersed objects possessing regular mesopores of the MCM-41 type; lengthening of the hydrophobic tail of the template resulted in smaller particles with greater intraparticle pores. The aggregation and sintering of individual silica particles during the calcination step led to the formation of particle clusters comprising interparticle voids, as evidenced by the ^{129}Xe NMR and TEM studies. The calcined particles were subsequently loaded with metallic silver. The measurements of iodine adsorption onto Ag-functionalized materials from the gas phase were supplemented by XRD, SEM/EDX, and TGA/DTA studies. It was demonstrated that the functionalized silica retained much gaseous iodine in an irreversible manner, mainly as an 'interfacial' AgI. The best compromise between the textural parameters and the post-synthesis functionalization was obtained for the large-pore silica templated with C_{18}TAB. Indications about the presence of silver metal nanoparticles, displaying certain heterogeneity in size and shape, within the pores of this sample were given based on the analysis of ^{129}Xe NMR spectra supplemented by UV-Visible absorption spectra and powder XRD patterns in the wide-angle region. The material can be recommended for the entrapment and immobilization of radioactive iodine in the nuclear industry since it guarantees that the adsorbed pollutant is primarily localized within the material pores and is thermally stable up to 800 K in air.

Key words: Mesoporous silica, gaseous iodine entrapment, Ag nanoparticles, ^{129}Xe NMR characterization.

Eriochrome Black T Adsorption Mechanism on Al_2O_3 Nanoparticles: Optimization and application to a Real Wastewater Effluent

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The Eriochrome Black T (EBT) adsorption onto Al_2O_3 nanoparticles has been investigated as a function of contact time, initial EBT concentration, and temperature. The experimental design method generated optimum conditions as tc = 40 min, 55 mg/L, and T = 298 K. The kinetics study was discussed using different kinetic models. The adsorption experiments of EBT show a better fit to the model pseudo second order (R^2=0.999). The experimental data were analyzed by different isotherm models. Freundlich's well-fitted modeling proved that the adsorption of EBT on Alumine occurred as multilayers and on a heterogeneous surface. The Thermodynamic study for the present process was performed by determining the values of ΔG°, ΔH°, and ΔS° indicate that the adsorption was spontaneous, physisorption and exothermic.

Graphical Abstract

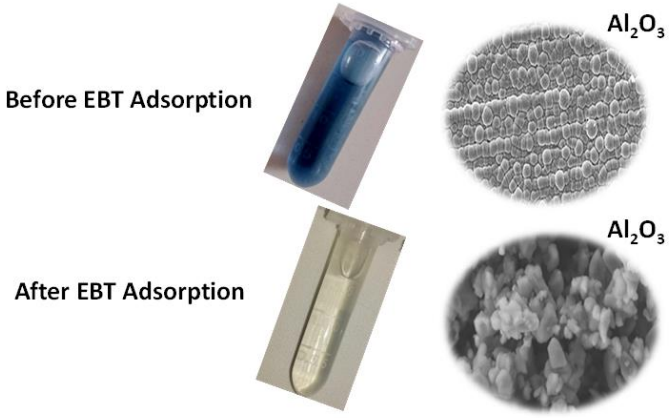

Figure: Effluent aspects and SEM micrographs before and after EBT adsorption onto Al_2O_3 nanoparticles at optimum conditions.

Synthesis and physico-chemical characterization of a new hybrid material based on perchloric acid and 3.4.DAP

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The hybrid compound with the formula $(C_5H_8N_3)ClO_4$ was elaborated in aqueous solution at room temperature by the slow evaporation method. It crystallizes in the monoclinic non-symmetric space group $P2_1$ with the following parameters: a=5.1261 (9), b= 9.3003 (17), c= 8.6659 (16) Å and β= 102.595 (7)°. However, the supramolecular crystal structure was built from perchlorate anions $(ClO_4)^-$ and organic diaminopyridinum cations $(C_5H_8N_3)^+$ connected with hydrogen bonds to form a three-dimensional network. The Fourier transform infrared (FTIR) and the Raman spectra indicate that the vibrational modes correspond to both inorganic and organic entities. According to the Hirshfeld's analysis, the crystal packing is mainly stabilized by the presence of hydrogen bonds O···H (50%). Furthermore, the thermal behavior was studied by thermogravimetric (TGA) and differential scanning calorimetry (DSC) appears to have good stability up to 268°C. Finally, optical properties were investigated by UV-Vis absorption and photoluminescence spectroscopy along with the discrete Fourier transform (DFT) theoretical calculations. This new compound exhibits lower cut-off energy and emission properties, with a band gap energy of 4.3 eV.

Physico-chemical characterization of *Spirulina Arthrospira platensis* and evaluation of its adsorption on hydroxyapatite

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Arthrospira platensis, better known as Spirulina (SP), is one of the most important microalgae species. It possesses a rich metabolite pattern, including high amounts of natural pigments. In this study, we applied a many strategy based on Fourier Transform Spectrometry (FTIR), Raman Spectroscopy, thermogravimetric Analysis (TGA) and Inductively Coupled Plasma analysis (ICP) for the characterization of Spirulina. The present contribution was aimed also at exploring SP/hydroxyapatite interactions. SP adsorption on a synthetic carbonated nano crystalline apatite characterized (by FTIR, Raman, TG-DTA) was investigated in detail, pointing out a good agreement with Sips isothermal features.

FTIR spectra of SP have been recorded in the region of 3428-3320 cm-1 to 620-490 cm-1 in the different frequency ranges. We obtained three Raman characteristic peaks through density functional. The TG curve indicated the existence of three main weight losses. The most relevance of inorganic micronutrients in SP is iron, magnesium, calcium, zinc, phosphorous, manganese, copper and chrome. They are important for nutrition human bone.

SP was found to adsorb effectively onto hydroxyapatite. Vibrational spectroscopy data (FTIR and Raman) pointed out spectral modifications up on adsorption, confirming chemical-like interactions between SP and hydroxyapatite. The present study is intended to serve as a basis for future research works involving SP and apatite nanocrystals/nanoparticles in view of biomedical applications.

Investigating the kinetics of a highly efficient photocatalytic process involving TiO_2-USY nanocomposites

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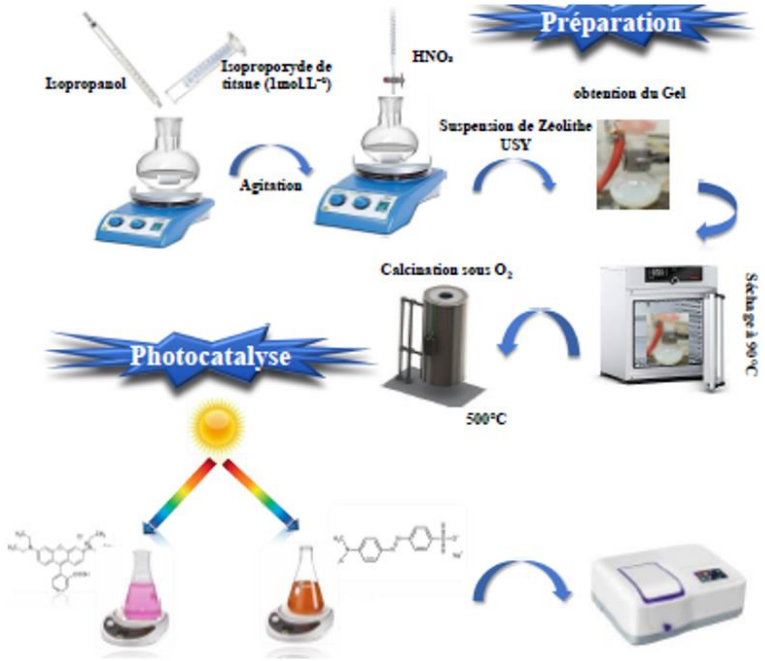
"Water is the structuring element of life. It is the structuring element of everything" *(R. Gafrej, 2023)*. One of the most main method for water depollution is the solar photocatalysis which using of a renewable energy. This technic attracted a great deal of attention thanks to its simplicity, low cost and non-toxicity. In addition, solar photocatalysis contributes to the reduction of greenhouse gas emissions associated with energy production. It thus offers a more environmentally-friendly solution and contributes to the fight against climate change.

Supported TiO_2 are very promising system for several types of pollutants, since the support allows for greater dispersion of the active sites. In fact, the integration of TiO_2 supported on zeolite combines the latter's adsorption capabilities with the former's photocatalytic activity, producing a synergistic effect that boosts photocatalytic efficiency.

The mains objectives of this work is to develop photocatalytic nanomaterials by combining TiO_2 with USY zeolite and the kinetic study of this system. We examined the effect of some parameters such as the contentent of TiO_2, the temperature of calcination, the time of the reaction and the type of the pollutant.

Based on these results, we can conclud that the loading on USY has an appreciable effect. We reach a degradation rate of 70% after 60 mn. This finding indicates that there is a synergistic effect between adsorption and textural properties of the support and photocatalytic behaviour of semi-conductor which confirms that this material type is a promising support for TiO_2 specially when it is prepared by sol-gel method.



Synthesis and ionic conductivity of phosphate and sulfate fluorapatites $Ca_{10}(PO_4)_6F_2$ and $Ca_4Na_6(SO_4)_6F_2$

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Phosphate and sulfate fluorapatites $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$ (x= 0, 6) have been synthesized by the solid-state reaction at high temperature. The samples have been characterized by X-ray Diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman scattering spectroscopy and Transmission Electron Microscopy (TEM) techniques. XRD study shows that these materials crystallize in the hexagonal system with $P6_3/m$ as a space group. An impedance analysis has been used to analyze the electrical behavior of the samples at different temperatures. Evidence of temperature-dependent electrical relaxation phenomena is observed. The bulk resistance decreases with increasing temperature, showing a typical negative temperature coefficient of resistance (NTCR). Ac-conductivity measurements have been performed on a wide range of frequencies and temperatures. The ionic conductivity follows the Arrhenius and the Jonscher laws.

Keywords: Fluorapatite; Complex impedance spectroscopy; Ionic conductivity; SOFC.

Synthesis and characterization of catalysts based on spinel oxides. Applications to the COPROX reaction

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CuAl2O4 prepared by auto-combustion has been examined with respect to its catalytic performance for preferential CO oxidation in a H2-rich stream. In turn, the promoting effects of incorporation of Ce by impregnation on the surface of CuAl2O4 on the process are examined as well. The catalyst have been characterized by ATG, X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), temperature programmed reduction (TPR), and X-ray photoelectron spectra (XPS), as well as diffuse reflectance infrared DRIFTS under reaction conditions with the aim of establishing structure/activity relationships for the mentioned catalyst/process.

Keywords: CuAl2O4 spinel; supported Ce; XRD; TEM; TPR; XPS fitting; CO-PROX; DRIFTS

Comparative characterization of the inhibiting properties of the mixture of Beetroot and Okra on mild steel in 0.5 M H2SO4 with molecular Dynamis simulation

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The extract of the mixture of Beetroot and Okra was the subject of our work in order to study their inhibitory efficiencies on mild steel and in the acid medium 0.5 M H2SO4. Several analytical methods were used, such as stationary electrochemical methods (potentiodynamic polarization), transient (Electrochemical Impedance Spectroscopy (EIS)) as well as the method of characterization of the surface of steel the Scanning Electron Microscopy (SEM). The inhibitory efficiencies obtained with the same concentration of 1000 ppm of the extract is 70%. The two green inhibitors act as a mixed inhibitor, with the polarization resistance values increasing with the increase of the inhibitor concentration. We are in the presence of physisorption for both inhibitors, in synergy. The characterization of the steel surface state confirms the results obtained.

Key words: Corrosion, Beet, EIS, okra, green inhibitor, mild steel

Optimisation of adsorption removal of Bisphenol A using sludge-based activated carbons: Application of response surface methodology with a Box–Behnken design

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In this work, the potential use of sewage sludge as a precursor for the production of activated carbon was explored. After chemical activation with $ZnCl_2$ three distinct activated carbon materials were obtained. These materials were employed to decontaminate synthetic solutions containing Bisphenol A and the results were compared with a commercial activated carbon. The effect of the impregnation ratio and the use of CO_2 on the textural properties and Bisphenol A adsorption performance were studied. The Kinetics of bisphenol A adsorption were successfully described by both pseudo-second order and Elovich models. While, the adsorption isotherms were well fitted to the Freundlich and Sips models. The prepared activated carbon had excellent adsorption efficiency toward bisphenol A with a maximum adsorption of 285,8 mg/g which was closer to the retention amount of the commercial one. To optimize the conditions for Bisphenol A removal, Response Surface Methodology (RSM) in coupled with the Box-Behnken design (BBD) was applied. Under these conditions, 657,7 mg/g can be reached.

Key words: Activated carbon; adsorption; sewage sludge; Bisphenol A; BBD; RSM.

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Enhancing Low-Temperature Formaldehyde Oxidation: Investigating Selectivity and Catalytic Activity of Co, Cr, Mo, and Ag Metal Catalysts Supported on γ-Al_2O_3

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Formaldehyde is a notorious indoor air pollutant that poses serious health risks with prolonged exposure. Catalytic oxidation at room temperature is an efficient approach to eliminating formaldehyde from indoor air. In this study, a series of 5% metal catalysts (Co, Cr, Mo, and Ag) supported on γ-Al_2O_3 were fabricated by a facile two-step synthesis method that included sol-gel and impregnation methods. The materials underwent characterization through a range of techniques, including XRD, TEM, FT-IR, BET, and H_2 -TPR. The catalytic activities and oxidation reactions of formaldehyde (HCHO) were examined using an analytical system equipped with an infrared analyser (MKS multigas 2030) to discern the various products. The resulting γ-Al_2O_3 catalysts obtained exhibited the diffraction peaks of the cubic structure of the γ-alumina phase, high surface area, and porosity. The physicochemical and catalytic properties of the catalysts, as well as the selectivity of by-products, were metal-dependent. Among the metal-based catalysts, the Ag/γ-Al_2O_3 catalyst exhibited excellent performance, achieving 100% formaldehyde conversion at 125°C with only CO_2 and water as by-products. The Co/γ-Al_2O_3 exhibited complete formaldehyde conversion with enhanced CO_2 selectivity at 250°C. TEM analysis of the Ag/γ-Al_2O_3 catalyst revealed well-dispersed silver particles on the support. These findings demonstrate the potential of metal-loaded γ-Al_2O_3 catalysts to effectively remove formaldehyde at low temperatures while maintaining high selectivity towards desired by-products. This information could pave the way for the development of high-performance catalysts at ambient temperatures.

Keywords : HCHO, γ-Al_2O_3, by-products, selectivity's, low temperature, Sol-Gel, metal supported

Exploring the sustainable and possible recycling of end-of-life tires to useful carbonaceous nanomaterials in water remediation

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This research was intended to produce useful products starting from end-of-life polymeric materials, such as spent tires, which generally degrade hardly, causing serious environmental problem. Pyrolysis is one of the eco-friendly methods that is used in the recycling of end-of-life tires which was performed in this research. The method was optimized to the best conditions to give different carbonaceous nanomaterials as the solid product, which was characterized by different characterization technics such as TEM, SEM and XRD to investigate their morphological structure and its composition. The results showed carbon dots in addition to different sizes of fullerenes, in the other hand, XRD showed presence of the calcite as a result of existing of calcium carbonate in the initial composition of the tires. These carbonaceous nanomaterials were used in the environmental protection application. Crystal violet is one of the toxic dyes, according to world health organization, and used in different applications such as textile and paper dye, this dye was removed be the resulted carbonaceous nanomaterials produced by the pyrolysis method, and the result showed very high removal capacity reach to 400 mg/g with two stages of removal and pseudo second order kinetic mechanism.

Key words

End-of- life tires, pyrolysis, crystal violet, fullerenes, carbon dots, carbonaceous nanomaterials.

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PHOTOCATALYTIC APPLICATION OF TiO_2 QUANTUM DOTS ASSEMBLED ON NANOSTRUCTURED TiO_2

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Among its many applications in the environmental and energy fields, TiO_2 photocatalysis is used for self-cleaning surfaces, air and water purification systems, sterilization, hydrogen evolution, and photoelectrochemical conversion. Recently, nanotechnology has demonstrated that nano-sized titanium dioxide photocatalysts, are highly effective in photodegrading organic and inorganic contaminants in water [1]. In fact, several approaches have been employed to formulate structures and electronic properties of TiO_2 at the nanocrystal level, including the control of the band structure, doping and heterojunction interaction [2-4]. In this work, we propose an alternative approach for constructing homojunctions between TiO_2 quantum dots (QDs) and titanium substrates. These homojunctions were characterized by X-ray diffraction (DRX), physisorption of nitrogen, photoluminescence excitation spectroscopy (PL) and UV-Visible spectroscopy. From the outcomes, the strong interfacial interaction between nanostructured TiO_2 and QDs efficiently reduces the recombination of photogenerated electron-hole pairs and enhances the charge transport [5]. In terms of catalytic application, TiO_2 catalysts showed high photocatalytic activity for the degradation of methylene blue present in water (up to 70% in 140 min).
Currently, efforts are being made to optimize and characterize other TiO_2-based catalysts, which exhibit promising performance and highlight alternative proposals and assumptions about QDs/support coupling. As a result of this work, a new vision of homojunctions based on quantum dots is being created, and new paths are being opened for practical applications of photocatalysis in the field of water treatment.

Key words: Heterogeneous photocatalysis, TiO_2, quantum dots, homojunction, water treatment.

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Potential pulse-assisted formation of aptamer/polydopamine double-layer onto gold nanoparticles modified electrode for sub-femtomolar capacitive detection of kanamycin

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The improper use of the kanamycin (KAN) antibiotic in the breeding sector has the potential to endanger human health by means of food contamination [1]. Therefore, it is crucial to monitor KAN levels in foodstuff like dairy products to ensure the overall health and safety of individuals. Increasing attention has been directed towards the utilization of aptasensors based on gold nanoparticles (AuNPs) for the quick and effective detection of KAN residue in food products [2].

In this context, we designed a capacitive-based biosensor for the detection of KAN at sub-femtomolar levels. Potential-pulse assisted method was used for the layer-by-layer electrodeposition of polydopamine (PDA) and KAN specific aptamer onto gold nanoparticles modified screen-printed carbon electrode. In the presence of kanamycin, the alteration of pseudocapacitive properties of PDA-modified electrode enabled label-free detection of this antibiotic with a linear response ranging from 2 fM to 206 pM and a limit of detection of 1.2 aM. Subsequently, the developed aptasensor was employed to detect KAN in fermented milk sample with good recovery, indicating its promising potential for analyzing antibiotic residues and ensuring food safety.

Key words: Capacitive detection, Aptasensor, Gold nanoparticles, Polydopamine, Kanamycin.

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Synergistic Co/Zr Composite Materials for Enhanced Antibacterial Activity: Sol-Gel Synthesis and Characterization

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Nano and micro-scale materials are gaining significant attention in the fields of medicine, pharmaceuticals, and antiseptic applications, showcasing their potential as antibacterial agents, imaging contrast elements, and carriers for drug and gene delivery into cancer-causing cells. This study focuses on the one-step sol-gel synthesis of Co/Zr composite materials to exploit the synergistic antibacterial properties of cobalt and zirconium, particularly against antibiotic-resistant bacteria. The investigation sheds light on the critical role of preparation conditions in achieving the desired material properties.

The sol-gel method was employed, resulting in the division of the gel into two parts. The first part underwent drying under atmospheric pressure in an oven, while the second part was dried under supercritical conditions. The effect of drying conditions on the properties of the resulting solids was meticulously studied. Notably, aerogels exhibited higher antibacterial activity against Gram-negative bacteria compared to xerogels, which demonstrated lesser activity against all tested bacteria.

The synthesized Co/Zr aerogels were further characterized using high-resolution scanning electron microscopy, energy-dispersive X-ray spectroscopy, and diffuse reflectance spectroscopy. The results revealed that the aerogels possessed a regular, spherical shape and were heavily aggregated into nanometric-sized clusters. In terms of antibacterial properties, the synthesized nanoparticles, referred to as Zr-doped Co-NPs, demonstrated heightened effectiveness against Escherichia coli and Klebsiella pneumoniae, with inhibition zones extending up to 15 mm at a concentration of 35 µg/mL. Similar results were observed against the Staphylococcus aureus strain at a higher concentration (45 µg/mL). However, no significant activity was observed against Enterococcus faecalis strains. The diverse structures and morphologies of the tested nanomaterials played a pivotal role in influencing their antibacterial capabilities, with aerogel particles characterized by a spherical form and nanometric size, while xerogel particles exhibited irregular shapes and larger sizes.

Gold-Modified Laser-Scribed Lettuce-Like Graphene Electrodes for Ultrasensitive Detection of Bioactive Molecules

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The imperative of overseeing levels of biologically active compounds in human body fluids, as well as their detection, holds a paramount significance in the context of human health monitoring for diverse applications such as drug analysis, pharmaceutical advancement, and environmental evaluation [1,2]. Notably, paracetamol (PCM), a frequently employed pharmacological ingredient in a variety of pain relievers and fever reducers, garnered high attention within this context [3]. Consequently, the ongoing pursuit of cost-effective and efficient sensors for PCM detection remains a dynamically evolving realm of research. In this study, we present a simple and effective approach to fabricate laser-induced graphene electrodes (LIGEs) through direct laser writing on a polyimide membrane. These LIGEs are further enhanced by functionalization with gold nanoparticles (AuNPs/LIGE). Through electrochemical investigations, we demonstrated that the addition of gold nanoparticles to the electrode surface led to notable improvements in both the electrochemical surface area and heterogeneous electron transfer rate. Moreover, the AuNPs/LIGEs exhibited the capability to accurately detect paracetamol even amidst various potential interferences and within the complex medium of human blood serum. Furthermore, the results showed that the AuNPs/LIGE platform is well-suited for paracetamol sensing within a linear range spanning from 5 to 2000 nM, with an impressive detection limit of 3.39 nM.

Key words: Laser-induced graphene, AuNPs, Sensor, Paracetamol, Electrochemistry.

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Electrochemical effect of spent coffee grounds extract as an eco-friendly inhibitor on copper corrosion in chloride media

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Potentiodynamic polarization and electrochemical impedance spectroscopy have been used to examine the inhibitory effect of aqueous extract of spent coffee grounds, SCG, on copper in NaCl 3%wt solution. The polarization curves around the OCP were fitted with various kinetic laws using a computer program to obtain detailed information about the inhibition process. A similar pattern was observed in the electrochemical tests. The corrosion current density decreased and the inhibition efficiency increased, as the extract concentration and time of immersion increased. The spent coffee grounds extract behaved as a cathodic-type inhibitor for copper in 3%wt NaCl solution.

Keywords: SCG, copper, voltammetry around OCP, EIS

Magnetic nanoparticle-based enzymatic biosensor for fluorescent detection of H_2O_2 in pasteurized milk

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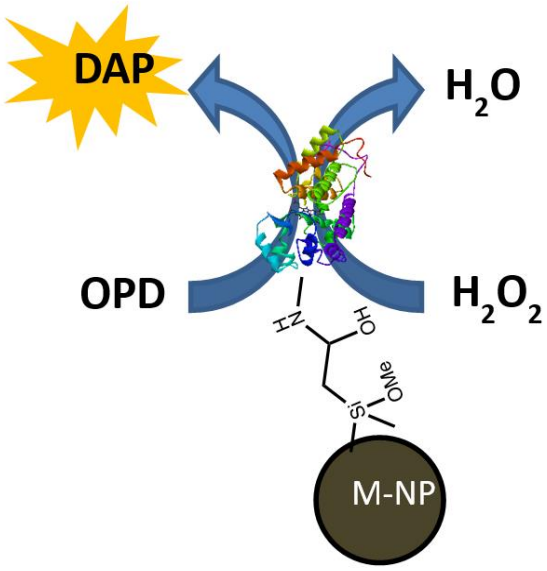
Hydrogen peroxide is an oxidizing agent used as sterilizing product in food production (milk, honey, juice…)[1]. At the end of the process, the dosage of H_2O_2 must not exceed the authorised limit value.

In this work, a novel fluorescent and enzymatic biosensor based on horseradish peroxidase (HRP) functionalized magnetic nanoparticles was developed to detect hydrogen peroxide as analyte in the presence of o-phenylenediamine in solution used as transducer. In fact, the oxidation of o-phenylenediamine (OPD) by H_2O_2 generate fluorescent 2,3-diaminophenazine (DAP).

The prepared biosensor showed a linear dependence between the fluorescence intensities of DAP and the concentration of H_2O_2 over the 10-30 µM range with a high sensitivity (0.0421 µmol/L). The influence of interfering species (ascorbic acid and glucose) is negligible, suggesting high selectivity of this bioplatform to the H_2O_2 target.

The proposed biosensor was also successfully used for hydrogen peroxide detection in pasteurized milk.



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Impact of the Ni and the Mg doping on the microstructure and the dielectric properties of $CaCu_{2,9-x}Ni_xMg_{0,1}Ti_4O_{12}$ ceramics

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$CaCu_3Ti_4O_{12}$ (CCTO) ceramics have significantly sparked a lot of research due to their high dielectric constant. It is considered potential materials for capacitor applications. However, its high dielectric loss (tanδ), which is greater than 0.1, makes it unsuitable for a lot of uses. Generally, CCTO doped with Ni ions exhibits exceptionnel dielectric constant properties and a high tanδ. The work focuses on improving the capacitor properties by simultaneously adding Ni and Mg to the lattice of copper titanate $CaCu_{2,9-x}Ni_xMg_{0,1}Ti_4O_{12}$ (with x = 0, 0.1, 0.15, and 0.2). All the ceramic samples were prepared by solid-state reactions. We found that the crystal structure of these sintered ceramics is identical to that of $CaCu_3Ti_4O_{12}$. The impact of the Ni and Mg on the structure and dielectric properties of CCTO ceramic was analyzed through X-ray diffraction, scanning electron microscopy, Raman, and dielectric measurements. The increase in Ni content brings about a decrease in mean grain size. The Raman and EDS measurements indicate the presence of CuO and MgO phases at grain boundaries. The dielectric constant values of ceramic samples range from 10^4 to 10^5. They decrease progressively with the addition of the Nickel, accompanied by a degradation in the dielectric loss. it remains higher than pure CCTO but lower than the compound doped only with Nickel. In view of these results we studied the impact of sintering process conditions on the structural properties. The results obtained confirm that increasing the calcination temperature while decreasing the time to 12 h has an insignificant effect on grain enlargement. The latter seem to have the same distribution but a slightly larger size. Electrical studies indicated that the internal barrier layer capacitor (IBLC) model is the most appropriate for the colossal dielectric response in these ceramics.

Keywords: Permittivité colossale, caractérisations électriques, condensateurs, céramiques, $CaCu_3Ti_4O_{12}$.

Microstructures and electrical properties of pure and chromium-doped $CaCu_3Ti_4O_{12}$ ceramics

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Pure and chromium-doped CCTO ($CaCu_3Ti_4O_{12}$) ceramics were prepared by a conventional solid-state reaction method. The effects of chromium doping and sintering time on the electrical properties of the CCCTO ceramics were investigated and discussed. X-ray diffraction studies (XRD) revealed that all samples exhibit a cubic perovskite single phase of type $CaCu_3Ti_4O_{12}$ (CCTO). But CuO and $CaTiO_3$ phases were also found. Scanning electron microscopy (SEM) results show that Cr doping suppressed the abnormal growth of grains, thus the grain size distribution became more uniform with the increase of Cr doping content. So the densification and the complex permittivity were affected. Both the addition of Cr and the longer sintering time of the as-prepared ceramics cause significantly affect the dielectric properties of the materials. The analysis revealed that the dielectric constant reached a value as high as $2\ 10^4$ (at 1 kHz) at a chromium-doping concentration of 3%. The dielectric study showed two major contributions associated with the grains and the grain boundaries. The analysis of the electric responses of these ceramics confirmed the occurrence of Maxwell–Wagner type relaxation, which is dependent on the frequency. These results suggest that the movement of oxygen vacancies at the grain boundaries is responsible for both the conduction and relaxation processes. The proposed explanation of the electric properties of pure and chromium-doped CCTO ceramics is supported by the data from the impedance spectrum.

Keywords: Permittivité colossale, caractérisations électriques, condensateurs, céramiques, $CaCu_3Ti_4O_{12}$.

DFT, X-Ray cristallography and NMR analysis of new β-phosphonated thiosemicarbazones crystals

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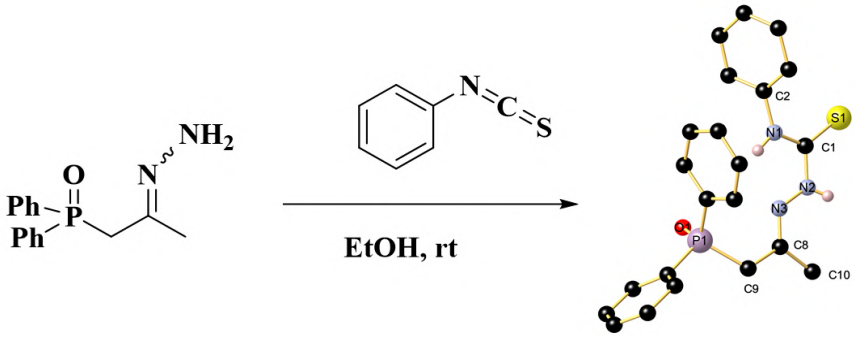
Thiosemicarbazone compounds[1] and their metal complexes exhibit noteworthy antiviral, antituberculous, antibacterial, and antitumor properties[2]. Consequently, the synthesis of novel thiosemicarbazone ligands holds both theoretical and practical importance. In this context, several phosphonated thiosemicarbazone ligands were synthesized by combining β-phosphonated hydrazones[3] with organic isothiocyanates, as outlined in Scheme 1.



All the synthesized products were structurally characterized using NMR spectroscopy, X-ray crystallography and DFT computing. An analysis of the crystal structures reveals the occurrence of intra- and intermolecular hydrogen bonding.

Keywords: Thiosemicarbazone, Crystal structures, DFT, X-Ray Crystallography

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Photo-Fenton Oxidation of Congo Red by a Heterogeneous Catalyst

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A heterogeneous catalyst was synthesized by surface modification of natural hematite using the simple impregnation method. The obtained catalyst was characterized by several techniques proving the surface modification of the hematite. The catalytic performance of prepared catalyst was evaluated in the Fenton type and Photo-Fenton oxidation of Congo red dye. The reactivity and stability of the catalyst was differentiated by studying the influence of the amount of used catalyst, leachate activity and catalyst reuse on the conversion of the initial concentration of Congo red. The oxidation of Congo red was studied under various experimental conditions. The best conversion rate of Congo red was about 89% using the catalyst under optimal conditions: $[H_2O_2]_0$ = 1 mmol/L, pH = 3, temperature = 25 °C. The impregnation method allows the preparation of an efficient and stable catalyst.

Keywords: Hematite - Congo red - Photo-Fenton.

CHEMICAL CHARACTERIZATION OF PARAFFIN DEPOSIT FROM PETROLEUM PRODUCTION AND PREVENTION METHODS

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Wax deposition is one of the most important flow assurance problems in the oil industry including the offshore and onshore oil fields. Indeed, paraffinic waxes present in petroleum crude can precipitate when temperature decreases below the wax appearance temperature. These deposits can result in significant financial losses through pipelines clogging and stopping production. For this reason, wax deposition brings severe challenges to the production, transportation, and storage of crude oils.

Therefore, it is essential to study and develop preventive strategies to control the formation of deposits in order to minimize the economic risks and maintain the continuity of crude oil production.

In this work we are interested in the case of an oil field in Tunisia, which produces a paraffinic crude. The exploitation of this field and the shipment of the produced oil to storage terminal, have led to the accumulation of deposits.

The characterization of the crude oil and the deposit formed has been done by several techniques included physical-chemical analyses (density, kinematic viscosity, pour point, asphaltenes content, paraffins content..), elemental analysis, chromatography, fourier transform infra-red spectroscopy, differential thermal analysis.

The obtained results have shown that the deposit is so rich in paraffin and characterized by higher asphaltenes contents than the original crude oil; and the paraffinic fraction isolated from the deposit seems to be of two types: microcrystals and macrocrystals.

In order to remedy the deposit problem, curative solutions have been used to dissolve the deposit. Several tests were performed by varying two parameters: chemical product injected content and temperature. The best results, for which deposit remained fluid at ambient temperature, were obtained by adding a dispersant of the paraffin deposit, previously mixed with a predetermined amount of the crude oil from which it is derived.

Finally, to find preventive solutions for reduce the paraffinic deposit formation, in order to ensure successful flow of the production stream from the reservoir to the point of sale, several tests were performed using different paraffin inhibitors.

Key words: Flow assurance, crude oil, paraffin deposit, preventive method.

The TiO_2/Ti_3C_2 MXenes structure in Toxic Metal Removal using Combined Batch/Electrochemical Processes: ADOX and OAP

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This work addresses a significant research gap by presenting the latest advancements in MXenes materials, including adsorbents and photo-catalysts, for selective separations in water treatment, specifically targeting the removal of heavy metals. Some hypotheses have been made using the TiO_2-Ti_3C_2 as MXene and the Cr and Cu as the toxic metal. These pollutants pose a grave environmental concern as they adversely impact the quality of water bodies, thereby affecting various living organisms. The work demonstrates the superior separation capabilities of MXenes materials in eliminating such toxic compounds. Additionally, MXene-based composites have garnered considerable interest as photo-catalysts for contaminant degradation due to their exceptional thermal and optical properties, hydrophilicity, substantial surface area, customizable chemical characteristics, high chemical stability, regular planar configurations, high metallic conductivity, and numerous derivative products. Literature highlights numerous MXene-based materials exhibiting fascinating separation performance when compared to other available two-dimensional (2D) materials. The potential of MXene-based composites in toxic metals removal is noteworthy; however, several challenges need to be addressed to enable their practical applications in real water environments.

Cerium and lanthanum detection using isosorbide-based poly(ether sulfone)

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Rare earth elements (REEs) are extremely useful in the development of advanced technologies, especially electronics. However, these materials can pose a serious environmental problem if they are used or eliminated inappropriately, and their effects are the subject of much research in the field of environmental toxicology. Our main aim is to develop impedimetric sensors able to detect the rare earth elements La and Ce by modifying a platinum electrode using four partially bio-sourced polymers developed for the selective and sensitive detection of these elements. These polymers were produced in good yields by the polycondensation of isosorbide-based poly(ether sulphone) synthesised with difluoride, diamine, dihydroxyl and bismaleimide oligomers. The poly (ether sulphone) dihydroxyl sensor showed the best analytical performance for the detection of La and Ce ions with a detection limit of 10^{-9} g/L, which is 10^4 times lower than that of capillary electrophoresis and C4D detection techniques coupled with CE.

Key words: Poly(ether sulfone), electrochemical impedance spectroscopy, Detection, rare earth elements.

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Synthesis of Hawthorn seeds hydrochar for determination of antibiotics substances in surface water using solid phase extraction and liquid chromatography

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Pharmaceuticals in water have been an environmental issue since the 1990s [1]. An important but often ignored aspect is the fate of antibiotic residues that reach the environment through different pathways because antibiotics are typically present in environmental water in low concentrations, ranging from µg L^{-1} to ng L^{-1}. Solid phase extraction of antibiotics and their determination by a high-performance liquid chromatography were considered. A hawthorn seeds hydrochar was synthesized and characterized by FTIR and MEB. An experimental design was applied for the optimization of the solid phase extraction process. The factors governing the extraction of the various antibiotics are sample volume, elution volume, and type of elution solvent. The optimal conditions were 50 mL of sample solution, 5 mL of elution solvent and methanol of type elution solvent. The separation was performed using isocratic elution with 24:76 acetonitrile: acidified water (pH = 4) and 0.4 % triethylamine. The antibiotics were identified by diode array detection. Recovery, linear range, limit of detection (LOD), and limit of quantification (LOQ) were calculated. Surface water samples from were analysed and recovery ranged between 70 and 90,12% with % RSD < 9,5.

Keywords: solid phase extraction (SPE), design experimental, hawthorn seeds hydrochar, antibiotics, HPLC-UV, surface water.

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Structural and spectroscopic investigations on $KMgPO_4$:Ln

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A series of ceramic materials with the chemical formula $KMPO_4$ (M= Mg, Mn, Ni, Cu) and $KMgPO_4$:Ln were obtained by the high-temperature dry process. X-ray powder diffraction (XDR) showed that the resulting pure phases crystallize as a function of the divalent metal in several crystalline systems. Infra-red spectroscopy was used to identify the nature of the P-O bonds in the coordination polyhedral. Scanning electron microscopy analysis confirms the existence of the constituent elements and the content of dopants incorporated into the crystalline matrix. Complex impedance spectroscopy has been used to assess the conductivity of the obtained compounds. The conduction within these materials is purely cationic in the temperature range [513-653K] and occurs by migration of the ions under the effect of thermal agitation. Materials doped with rare earth ions have low activation energies and are therefore good candidates for electrochemical applications in magnesium-based batteries.

Keywords: Phosphate compounds, Electrode materials, Activation energies, Rare earths, Relaxation process.

Synergistic Antioxidant Properties of Cinnamon Essential Oil and Zinc-Exchanged Interstratified Illite-Smectite

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This research investigates the synergistic antioxidant properties resulting from the combination of cinnamon bark essential oil (CEO) and Tunisian clay exchanged with zinc (H-Zn). The CEO was extracted through steam distillation using a Clevenger-type apparatus, and its chemical composition was determined through Gas Chromatography-Mass Spectroscopy (GC-MS). Sodium (H-Na) used as reference and zinc (H-Zn) samples were obtained by exchanging NaCl and $ZnCl_2$, respectively. These modified clays were characterized using X-ray Fluorescence (XRF), X-ray Diffraction (XRD) and cation exchange capacity. The hybrid materials were prepared through simple adsorption of CEO onto H-Na and H-Zn.

The GC-MS analysis of CEO revealed the presence of six components, accounting for 100% of the total composition. The major component identified was cinnamaldehyde (97.475%), along with endobornyl acetate (1.134%) and δ-cadinene (0.603%). Results from GC-FID chromatography demonstrated that the maximum CEO adsorption reached approximately 45 mg/g on H-Na and 100 mg/g on H-Zn, respectively. The antioxidant activity of the prepared materials, along with free CEO, was evaluated using the DPPH (2,2-diphenyl-1-picrylhydrazyl) method. The findings indicate that the antioxidant activity of cinnamon essential oil remains unaffected by its encapsulation in clay. Moreover, the exchanged clays exhibit intriguing antioxidant properties, making them suitable for concurrent use with the essential oil. This study highlights the potential for utilizing the combined antioxidant effects of CEO and zinc-exchanged clay in various applications. The synergy between these materials offers a promising avenue for developing antioxidant solutions in areas such as food preservation, cosmetics, and environmental protection.

Thermochemical and kinetic study of the σ-hole bonding leading to I_2 and 4-(Dimethylamino) pyridine complexes in solution at 25°C

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A C-80 microcalorimeter was used to study the thermochemical and kinetic aspect of the formation of iodine (I_2) and 4-(Dimethylamino) pyridine (DMAP) complexes in solution at 25°C. First, a theoretical approach of the σ-hole bonding leading to these complexes based on the calculation of complexation energy values, $Vs_{min,max}$, localization of the molecular orbitals and the amount of charge transfer, was developed. The hexane was chosen as a solvent for both DMAP and I_2 solids. The plots of the complexation heats as a function of r = [DMAP]/[I_2] ratio (where [DMAP] and [I_2] are the concentrations of DMAP and I_2, respectively) show that the molar complexation heat decreases to a minimum value and increases. For particular r values we can suggest complex forms for the reaction between I_2 and DMAP by taking into account the measured and calculated complexation energies. The kinetic mechanisms and theoretical heat flow equations have been proposed for the lowest and highest r ratio. Iterating the heat flow equations while considering the deconvoluted curves allows to deduce the kinetic and thermodynamic parameters as: global order, partial order, rate constant, apparent rate constant, and complexation enthalpies: For each mechanism, the latter parameter agrees with both the measured and theoretical ones [1].

Keywords: Microcalorimetry, Thermochemical, kinetic, σ-hole bonding,
I_2 - 4-(Dimethylamino) pyridine complexes, DFT calculations

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Hydrothermal Synthesis of $(C_5H_{14}N_2)[CoCl_4].0.5H_2O$ Crystal Structure, Hirshfeld Surface, Antibacterial Activity and Magnetic Properties

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Single crystals of 1-methylpiperazine-1,4-diium tetrachloridocobaltate(II) hemihydrate, $(C_5H_{14}N_2)[CoCl_4].0.5H_2O$, I, were grown by hydrothermal techniques in aqueous solution. The X-ray diffraction analysis revealed that the compound crystallizes in the centrosymmetric space group C2/c of the monoclinic system. The crystal structure of the Co(II) complex is built from isolated [CoCl4]2– anions, 1-methylpiperazine-1,4-diium [C5H14N2]2+ cations, and water molecules which are connected in a 3-D hydrogen-bonded network. Hirshfeld surface analysis revealed that Cl···H/H···Cl and H···H (58.5 and 36.4 %, respectively) are the most significant interactions between species. Minor O···H/H···O interactions are also present. The thermal decomposition was studied by TGA-DTA techniques. Magnetic measurements indicate the presence of single-ion anisotropy and very weak antiferromagnetic interactions in the compound. The bioassay results showed that the compound exhibits modest antibacterial activity.

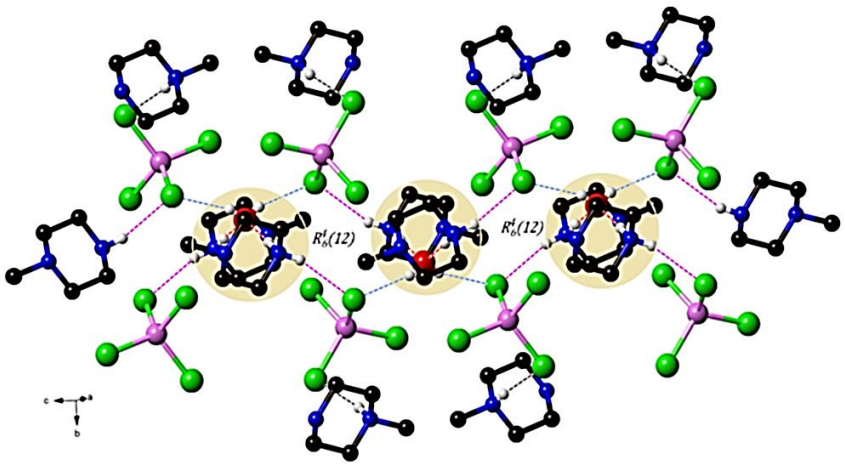

Figure: One layer showing the anions and cations···water interactions forming alternating $R_6^4(12)$ring motifs.

Catalytic treatment of wastewater

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The objective of this work was to study the wet oxidation reaction catalyzed with metal catalysts based on iron supported on Zirconia oxide and bimetallic catalysts based on cobalt andiron deposited on ZrO2, in order to degrade one of the endocrine disruptors: Triclosan. In this study, we used the sol-gel route for the development of aerogel supports. These supports are subsequently used to prepare a series of catalysts based on iron alone or iron and cobalt with fixed percentages by dry impregnation. All these catalysts are reduced under a flow of hydrogenat 300°C. The study of the textural and structural properties of the solids was carried out by measuring the specific surface area by the BET method and by TPR. The N2 adsorption-desorptionanalysis of the different solids shows similar isotherms with the ZrO2 support, with varied hysteresis loops which reflects different textures and porous distributions. The TPR-H2 profiles show the non-reducibility of ZrO2. TPR analysis of the catalysts shows peaks characteristic of thereduction of iron and cobalt. The results of the catalytic tests show that the monometallic iron- based catalyst supported on ZrO2, the bimetallic catalyst impregnated simultaneously on the ZrO2 support and the product X present significant catalytic activity in the degradation of Triclosan. This seems to be due to an increase in the average diameter of the pores and the pore volume which results in better iron-support interaction and therefore good dispersion of the metallic phase on the ZrO2 surface. The use of these catalysts and a product X for the catalytic treatment of ONAS wastewater showed their effectiveness to different degrees. * As perspectives: This study will be supplemented by other work on product X which should be further analyzed with a view to obtaining a patent which highlights it and encourages manufacturers to use it as a catalyst in the treatment Wastewater.

Effects of ultrasound technology parameters on phenolics and enzymatic activity in *Chemlali* and *Memecik cv*. olive paste.

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It is believed that describing the effects of high-power ultrasound applications on olive paste before malaxation will exhibit possible benefits for the future of olive processing technology. The experiment consists in the sonication treatment of *Chemlali* and *Memecik cv*. olive paste with different times (0,4, 8, 10 min). This kind of approach has never been used on of the degradation of phenolics during extraction. Taking into account the treatment time, the maximum of total phenolic compounds was reached after 10 min of treatment for Chemlali variety 60% is detected if olive paste without stones is used. On the other hand, the total phenolic content of *Memecik* cv. increases positively with the increasing time of treatment. Significant decreases in peroxidase and β-glucosidase activities were detected during increasing US treatment times, while our data showed that PPO activity increase more significantly in the case of depitted than that treatment of whole olive paste. Overall the results showed that ultrasound treatment of depitted olive paste has a high significant effect on the phenolic composition qua.ntified in both olive pastes from the two studied cultivars more than in those found from whole olive samples.

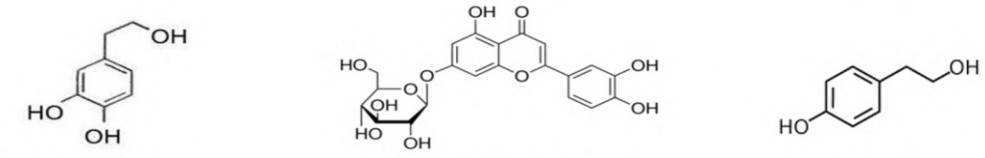

Fig. Major phenolic compounds identified in olive paste with regard to ultrasound pretreatment.

Key words: olive paste, phenolic compounds, sonication treatment, PPO activity.

Electrical characterization of silicon PV- cell: Modeling

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Under darkness and 100 mW/cm^2 illumination, a monocrystalline solar cell device's current-voltage properties were examined. According to AM1.5, the studied solar cell has an efficiency rate of 14.22% to70.2 relative to industry standards. Under both dark and light conditions, the electrical characteristics (capacitance, current-voltage, power-voltage, the transient photovoltage, the transient photocurrent and impedance) of a silicon solar cell device were examined. Under complete darkness and light intensity of 100 mW/cm^2 respectively, we have noticed that the light of AM1.5 spectrum changes the all PV-cell parameters such as short current, open circuit voltage, maximum power, maximum voltage and power conversion efficiency. Modern electrical and optoelectronic devices can benefit from the constructed mono-silicon solar cell device as photocapacitive and photoresistive component. By using a MATLAB programs, we have modelled the current versus voltage and power versus voltage properties of equivalent solar cell circuits, a good accordance between the experimental and theoretical curves.

Keywords: Silicon Solar Cell, Nyquist diagram, Electricals characteristics; Matlab programs.

Preparation of Bio-coagulant from Oak Leaves for Natural Waters Treatment

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Coagulants are used to clarify water by aggregating suspended particles. Since these chemical substances are often synthetic and can have negative environmental impacts, bio-coagulants received attention due to their eco-friendly nature and their efficiency. In this work, the bio-coagulant was prepared by grinding Canary Island oak leaves into powder. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Fourier Transform Infrared spectroscopy (FTIR) were performed for the structural and morphological characterizations of the prepared bio-coagulant. The application of Powdered oak leaves as a bio-coagulant was evaluated in batch coagulation-flocculation experiments for several natural waters. Experimental results showed that the bio-coagulant was efficient in removing turbidity, suspended solid (SS) and different minerals such as calcium, magnesium, and iron with removal yields up to 90% in optimal conditions. These results suggest that the bio-coagulant could be used as an alternative to the widely used coagulant to improve the overall quality of drinking water.

Keywords: Bio-coagulant, Preparation, Oak leaves, Characterization, Natural water treatment.

Water Absorption of HDPE/Washingtonia Filifera Fiber Biocomposites: Modeling Using GA-ANN

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The present study aims to investigate the phenomenon of water absorption scattering mechanisms and biocomposite kinetics by the immersion of different HDPE matrix reinforced with different amounts of *Washingtonia palm* (WP) fibers (10, 20, and 30% by mass) in distilled water at room temperature. Artificial neural network (ANN) model with genetic algorithm (GA) were examined by considering WP fiber content and immersion time in the water absorption of HDPE/WF biocomposite. The process of water absorption was revealed to be tracking the diffusion mode of Fickian. The results obtained show that the addition of WP fibers to HDPE matrix reduced diffusivity. The results also reveal that ANN models were highly accurate in the prediction of water absorption with the training, validation, and test correlation coefficients of 0.9866, 0.9889, and 0.9919, respectively. The optimal conditions obtained by GA for minimum absorption were a fiber content of 12% and an immersion time of 2 hours. Moreover, a highly appropriate model to predict HDPE/WP biocomposites water absorption suitable for various industrial applications is proposed.

Key words: Washingtonia palm fiber, HDPE matrix; Water absorption, Fick model, ANN.

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Hydrothermal synthesis and electrochemical properties of VO_2(B) nanowires as a cathode material

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Rechargeable lithium-ion batteries (LIBs) have been widely used as power sources for portable electronics, electric vehicles (EV), and hybrid vehicles (HEV) [1]. Among the various candidate cathode materials, vanadium oxides have attracted great attentions due to their high energy density, low cost, and abundant sources. In particular, metastable VO_2(B) stands out from these vanadium oxides because of its unique bilayer structure, large lattice spacing of edge-sharing VO_6 octahedron, high theoretical capacity, and fast ion-transfer rate [2,3].

In the present study, VO_2(B) nanowires were successfully synthesized by a facile one-step hydrothermal process using V_2O_5 and 3-aminopropanol as a precursor. The structural properties and the phase identification of VO_2(B) were investigated by X-ray diffraction (XRD). The morphological properties of the samples have been determined by scanning electron microscopy (SEM). The optical band gap of VO_2(B) was found to be 3.61 eV. In order to investigate the kinetics of reaction in electrode material, cyclic voltammetry curves were carried out at various scan rates from 5 to 50 mVs^{-1}. It has been found that peak currents (Ip) follow a power law relationship with the sweep rate. The results indicate that the reaction is controlled by a mixture of two contributions: charge transfer process and diffusion process.

Key words: hydrothermal treatment, lithium-ion batteries; VO_2(B); energy storage.

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Synthesis, optical and electrical properties of nano-V_4O_9 plate-like morphology

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In the past decades, nanostructured based vanadium oxide materials have been at the forefront of applied research because of their unique properties, which are different from their bulk materials [1]. In fact, solid state vanadium gives high current at oxidation states +3 to +5, leads to interesting physical and chemical properties and a wide range of potential applications [2].

The present communication reports the hydrothermal synthesize of V_4O_9 plate-like nanostructure, using V_2O_5 as vanadium source and 3-amino-1-propanol as reducing and structure-directing agent. The electrical conductivity and dielectric properties of was also studied using complex impedance spectroscopy. The structural and morphological properties of the nano-V_4O_9 were investigated by X-ray diffraction (XRD), infrared spectroscopy and scanning electron microscopy (SEM). The complex impedance data have revealed the presence of single relaxation associated with the grain effect. Furthermore, the depressed semicircles suggest the relaxation to be of a non-Debye-type.

The frequency dependence of AC conductivity at different tends to be constant while at higher frequencies it becomes frequency dependent, which can be explained in terms of Jonscher's laws. The CBH model is the probable mechanism for the AC conduction behavior. The conductivity was measured by complex impedance spectroscopy which is equal to 1.244 10^{-4} S. cm^{-1} at 298 K.

Key words: hydrothermal synthesis; nano-V_4O_9 plate-like; electrical properties; impedance spectroscopy.

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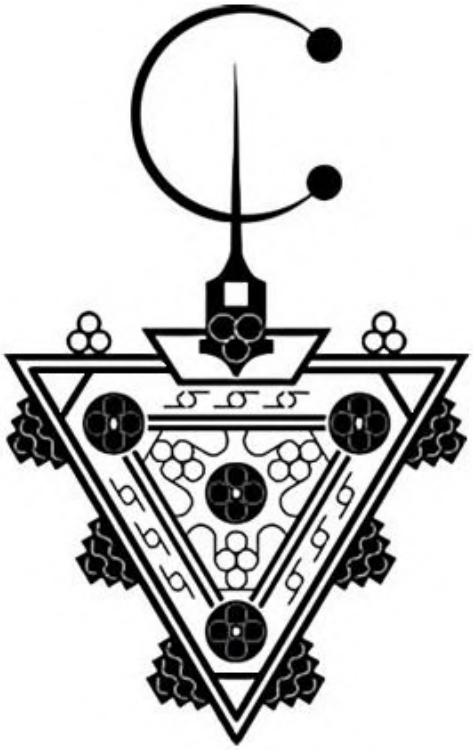

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