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13ème édition des Rencontres Marocaines sur la Chimie de l'Etat Solide
(REMCES 13)

Faculté des Sciences El Jadida

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Ecole Nationale
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15, 16 et 17 mai 2024, Université Chouaib Doukkali, El Jadida, Maroc
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13ème édition des Rencontres Marocaines sur la Chimie de l'Etat Solide
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Pour projeter la 13ème édition des REMCES sur des dimensions scientifiques dignes des aspirations des partenaires, collaborateurs et sponsors, le comité scientifique des REMCES a retenu 228 projets comptant 77 communications orales et 151 communications par affiche qui se rattachent tous aux thèmes de la rencontre. Ses projets affectés aux sessions thématiques correspondantes seront systématiquement précédés par des conférences thématiques. Un total de 12 conférences plénières et de 4 conférences programmées pendant les trois journées de la rencontre seront animées par des professeurs reconnus par la pertinence de leurs travaux de recherche. Les membres du comité local très satisfaits des échanges fructueux tenus avec tous les participants depuis la soumission des projets, tiennent à les remercier et à leur souhaiter beaucoup de succès dans la présentation de leurs interventions. Les membres du comité local profitent aussi de l'occasion pour rendre hommage à tous les conférenciers qui n'ont ménagé aucun effort pour prendre part à cette édition et contribuer à sa réussite.

Pour faire valoir les travaux de recherche présentés pendant les journées de la 13ème édition des REMCES auprès de la communauté scientifique internationale, il est proposé aux participants trois choix de revues scientifiques indexées pour la publication de leurs résultats. Les éditeurs et équipes des revues *Comptes Rendus Chimie*, *Environmental Sciences and Pollution Research* et *Moroccan Journal of Chemistry*, n'ont pas hésité à formuler l'avis favorable pour produire des numéros spéciaux sur les actes de la 13ème édition des REMCES, qu'ils acceptent les expressions de notre gratitude et de notre reconnaissance.

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C.P. 1

La Physique des Atomes de Rydberg

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Les propriétés exagérées des atomes de Rydberg (taille énorme, durée de vie très longue) les rendent extrêmement sensibles à leur environnement. Ces atomes géants peuvent maintenant être préparés et manipulés par excitation laser avec une grande précision. Ils interagissent très fortement avec les photons micro-ondes et entre eux, à des distances énormes à l'échelle atomique. Ces caractéristiques en font des outils idéaux pour explorer les phénomènes quantiques fondamentaux, pour construire des portes quantiques et pour réaliser des simulateurs quantiques de systèmes de matière condensée. Je rappellerai les débuts de la physique des atomes de Rydberg et décrirai des études récentes dans lesquelles des réseaux d'atomes de Rydberg interagissent les uns avec les autres de manière contrôlée, ouvrant des perspectives prometteuses dans la science de l'information quantique.

C.P. 2

Single-atom catalysts for energy conversion reactions

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Single-atom catalysis, a new concept coined in 2011 by our group[1], has emerged as one of the most active frontiers in catalysis. With the great potential for maximizing the atom efficacy and offering distinctive activity/selectivity in a variety of important reactions, single-atom catalysts (SACs) have received incredibly increased attentions from both academia and industry. In this presentation, I will introduce the fast progress of SACs in the recent years and address some of the fundamental issues about single-atom catalysis,[2-14] such as the nature of the active sites in SACs, the essential role of coordination structure of single atoms in catalysis, the dynamics of SACs during reaction, as well as the applications in the energy conversion reactions.

Keywords: Single-atom catalysis; nano-catalysis; supported metal catalysts; metal-support interaction; coordination environment; energy conversion.

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C.P. 3

Advanced functionalised materials for nonlinear optical applications

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Advanced functionalised Nonlinear Optical Materials are materials with specific nonlinear optical (NLO) properties that are widely used in photonics, nanophotonics devices. Interest in using the powerful tool for diagnostic of NLO properties of such specific multifunctional materials for nonlinear optics and nanophothonics applications are growing very rapidly and play a major role in emerging photonic technology. Nonlinear optics play a major role in many of the optical applications. Innovative optoelectronic devices for communications, optical switching, optical data information storage and optical limiting require an important development of materials based on molecular engineering of advanced molecular systems with exceptional NLO responses [1,3]. Thus, organic materials, polymeric materials, organometallic or coordination metallic complexes as well as new hybrid organic/inorganic nanocomposites have been the subject of both experimental and theoretical investigations during last recent years because of their valuable potential applications in photonics and optical devices and in the current development stage of advanced photonics technologies. There is great interest in the development of such photonics systems including self-assembled architectures for nonlinear optical applications and optoelectronics applications [2-5]. Molecular engineering is crucial for obtaining new photonics self-assembled architectures such as highly conjugated compounds based on supramolecular systems chemistry. Consequently, in this talk NLO properties of highly conjugated compounds based on supramolecular chemistry will be also discussed in view of their optoelectronics applications[4] using powerful experimental techniques tools such as SHG, THG, and Z-Scan. Moreover some interesting experimental results on anisotropic confinement of chromophores that induces second-order nonlinear optics in a nanoporous photonic metamaterial will be also discussed. The obtained properties provide a unique assemblage for exploring interactions in newly designed smart membranes.

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C.P. 4

Development of advanced Li/Na -ion batteries and beyond to reduce cost and ensure sustainability for electric vehicles.

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To meet the high-energy requirement that can enable the 40-miles electric drive Plug in Hybrid Electric Vehicle (P-HEVs), long range electric vehicle (EV) and smart grid, it is necessary to develop very high energy and high-power cathodes and anodes that when combined in a battery system must offer over 1,000 charge-depleting cycles, 15years calendar life as well as excellent abuse tolerance. These challenging requirements make it difficult for conventional battery systems to be adopted in P-HEVs and EVs. In this talk, we will first introduce the next generation lithium-ion battery that include Ni rich full gradient cathode with Nano-rode primary particles, a novel advanced PEDOT coating to extend the calendar life of battery, a high voltage and non-flammable Fluorinated based electrolytes and Silicon-graphene composite anode including a novel pre-lithiation technology to overcome the irreversible loss of this anode in the first cycle. We will also address the sustainability of the battery by showing a novel Na ion battery with a very high energy doped red phosphorus. We will then finish by describing a novel high energy SeS system with new electrolyte that suppress the dissolution of polysulfide species and eliminate the shuttle effect. This electrolyte is highly compatible with lithium metal anode.

C.P. 5

Enhancing Hydrogen Production via Photoelectrochemical Water Splitting: Innovative Photoanode Design Strategies for Superior Efficiency

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Facing the dual challenges of an energy crisis and escalating environmental concerns due to fossil fuel dependency, the scientific community is turning towards alternative, clean energy sources, with hydrogen emerging as a promising candidate. This talk will explore advanced strategies in photoelectrochemical (PEC) water splitting, particularly focusing on the innovative use of one-dimensional cadmium sulfide (CdS) or $BiVO_4$ nanoarrays as photoanodes to enhance hydrogen production efficiently and sustainably. It addresses the challenges of charge carrier recombination and photocorrosion in CdS or $BiVO_4$ nanoarrays by introducing novel design strategies like Type-I, Z-scheme, and plasmon-enhanced heterostructures, alongside $BiVO_4/MoS_2$ nanoarray architectures for improved charge separation. This exploration not only highlights the potential of these advanced PEC systems in advancing hydrogen production technologies but also emphasizes their role in moving towards a sustainable energy future.

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C.P. 6

Magnetocaloric Materials Based on Rare Earth Mixed Oxides

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During the last two decades the energy demand has increased exponentially, this could be due to the constant population increase, improving the standard living, economic growth, etc. Within this context the refrigeration and air conditioning processes account 20% of the total electricity power which represents 2000TWh. If the energy efficiencies of the systems used for the purpose are not improved or new technologies are not introduced the electricity consumption should be three times higher in 2050. In this sense, the research on magnetocaloric materials has attracted worldwide interest in recent years [1], due their high potential use for magnetic refrigeration in the low temperature range with the aim of liquefying He, H_2, or natural gas as an alternative technology to the traditional cooling systems based on of gas compression and expansion cycles [2].

Herein we include the study of the magnetocaloric effect (MCE) of three families of compounds: the tetragonal $R\mathrm{CrO}_4$ (R=rare earth) zircon-type oxides (S.G. $I4_1/amd$)[3], ,$(\mathrm{Mn}_{0.66}R_{1.34})(\mathrm{Mn}_{0.66}\mathrm{Sb}_{1.34})\mathrm{O}_7$ [4] and $R_2\mathrm{Ti}_2\mathrm{O}_7$ pyrochlores (Fd-3m), and $R_3M\mathrm{O}_7$ (M = Nb and Ta), (Cmcm) weberites. Magnetization, heat capacity and direct measurements of the magnetocaloric effect (MCE) show that $R\mathrm{CrO}_4$ zircon polymorph have a remarkable MCE at cryogenic temperatures [5]. Zircons have a large MCE near their Curie point, $T_C \simeq 20$ K, reaching maximum isothermal entropy increments, $|\Delta S_T| = 29$, 21, 19.4, and 16.2 J kg^{-1} K^{-1} for GdCrO_4, HoCrO_4, ErCrO_4, and TbCrO_4, respectively, under an external field of 5 T [4,5].The results, show large entropies up to 20.7, 11.3, 11.7 and 12.5 J kg^{-1} K^{-1} for $\mathrm{Mn}_{1.33}R_{1.33}\mathrm{Sb}_{1.33}\mathrm{O}_7$ pyrochlores with R = Gd, Dy, Ho and Er respectively in the 2-30K temperature range; 17.2 J kg^{-1} K^{-1} for $\mathrm{Tb}_2\mathrm{Ti}_2\mathrm{O}_7$ at 2 K, and 11.2 J kg^{-1} K^{-1} for $\mathrm{Tb}_3\mathrm{TaO}_7$ at 3K. These results provide a broad range of magnetocaloric properties, suggesting a new field of applications for these materials as magnetic refrigerants at cryogenic temperatures.

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C.P. 7

Elemental characterization on cultural heritage materials using x-ray spectrometry

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This work summarizes the results in the research on Cultural Heritage pieces with portable and non-portable X Ray Fluorescence and microbeam systems. Physicochemical study of parchment and paper of historical documents was carried on, in order to provide the characterization of the parchment, pigments and metallic coatings used in old manuscripts and illuminations for preservation and conservation perspectives. Non-destructive analysis was carried out in situ by Energy Dispersive X-ray Fluorescence (EDXRF) with portable instrument, for elemental composition[1,2,3].

With the aim of tracing differences in manufacturing techniques of glazed ceramics, several glazed ceramic fragments (XVI-XVIII centuries) from two production centers in Portugal were object of study. The system glaze/decoration is not easy to investigate, due to high heterogeneity of the mixing products and the diffusion ability of the pigment into the base glaze. It is variable depending on the composition both from the pigment and the glaze in terms of fusibility. Micro X-ray fluorescence analysis is the best choice to monitor the profile of the elements characteristic of the used colors and the thickness of the glaze. Cross sections performed on several fragments were carried out. By monitoring the profile of the characteristic element, we could identify diffusion from the pigment through the base glaze, the thickness of the glaze and the pigment corresponding to each color[4].

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C.P. 8

Design and fabrication of Relaxor-PT single crystals-based devices

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After enhanced the piezoelectric performances of PMNT and PIMNT single crystals by AC poling technique, two kinds of relaxor-PT based 3MHz phased array transducers have been designed by FEM simulation with PizeoFlex, then they have been fabricated with well performances, one has got the bandwidth 91.41%@-6dB and insertion loss -45.5dB by using three matching layers, anther has got the bandwidth 88.12%@-6dB and -32.46 by using de-matching layers, much higher performances compared with conventional PZT transducers. These single crystal transfers have higher resolution, deeper penetration depth for medical ultrasound imaging.

By doing Mn2+, the comprehensive pyroelectric and dielectric performances of PMNT and PIMNT single crystals have been enhanced for 12×10-4Cm-2K-1 pyroelectric coefficient, 0.05%@1kHz dielectric loss, and 40.2×10-5Pa-1/2 FOM for detectivity (Fd), much higher pyroelectric performances than conventional $LiTaO_3$ single crystal. Novel single element detector, and dual compensated pyroelectric detectors have been fabricated with detectivity D*～2×109 cmHz1/2/W@5Hz, 6 times higher than conventional LiTaO3 pyroelectric detector. Based on the novel pyroelectric detectors, NDIR gas detectors have been designed and fabricated to measure the concentration of various gases, such as CO_2 CO and CH_4.

ME composite PMNT/Metglas has been fabricated with ME charge coupling αQ~6200pC/Oe，capacity Cp~399pF，dielectric loss D~0.5%. Based on ME composite，ME magnetic sensors were designed and fabricated with the performances of sensitivity 0.8 pT/Hz1/2@1Hz, 0.2pT/Hz1/2@100Hz, 9fT/Hz1/2@EMR, power 20mW, and bandwidth 0.1Hz~15kHz, which are much better than conventional flux gate. Such novel magnetic sensors could be used in many areas for sensing magnetic field.

C.P. 9

Crystalline and Vitreous Inorganic Metal Phosphates Synthesis, Structural Characterizations and Properties

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University Hassan II, Faculty of Sciences Ben M'Sik, Casablanca, Morocco

Metal phosphates in both crystalline and glassy forms are extensively studied for their applications in renewable energy, biomedical engineering, and environmental remediation. They can be used as cathodes in lithium ion batteries, as lasers and light emitting diodes components, as sunscreens for UV radiation absorption, as pigments, as biomaterials, and last but not less, as hosts for nuclear wastes. The diverse properties and applications of phosphates depend on their structure, which is based on [PO4] tetrahedra. These tetrahedra can be isolated or connected to each other by sharing corners to form condensed phosphates. To illustrate the relationships between structure and properties of phosphates, this presentation will focus on examples of compounds in which [PO4] tetrahedra are connected with [MOn] polyhedra (M is a metal and n its coordination number). After enhanced the piezoelectric performances of PMNT and PIMNT single crystals by AC

C.P. 10

Structure and Dynamics of Chirality-Transfer Complexes on a Catalyst Surface

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Control of enantioselection is an especially demanding challenge in heterogeneous catalysis and its study explores phenomena ranging from ligand-induced rate-enhancement to the interplay between chemisorption and intermolecular forces in determining the structure and dynamics of chirality transfer complexes. In this study, a combination of STM, DFT and reflectance-IR data is used to define the structure of individual chirality transfer complexes, the intermolecular interactions involved, the activation of prochiral functional groups, and complexation state changes within isolated complexes. Although the studies are carried out on model systems under vacuum conditions, the observed phenomena are largely consistent with the operando heterogeneous asymmetric catalysis literature. Emphasis will be placed on the three most important insights gained from studies of single complexes formed by (R)-(+)-1-(1-naphthyl)ethylamine and activated ketones on Pt(111): (i) complexation is driven by multiple attractive non-covalent interactions; (ii) weak non-covalent interactions play a determining role in stereodirection; (iii) precursor state dynamics are key to forming privileged complexation structures. The studies also show that DFT calculations perform well in predicting the structure and dynamics of individual chemisorbed chirality transfer complexes.

C.P. 11

High Energetic Materials (HEM): synthesis, applications and safety

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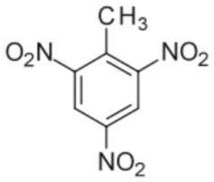
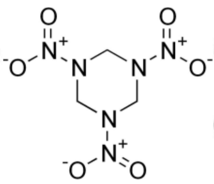
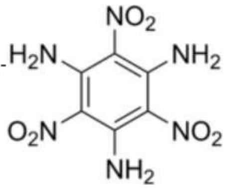
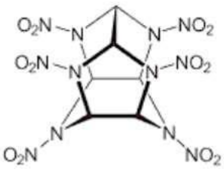
Energetic Materials (EM) are a class of materials which contains high amount of chemical energy stored in their molecular structure. Upon external stimulations, such as heat, shock, or electrical discharge, the energy can be released at different timescales, from fuel combustion to detonation (up to 9 km s^{-1} for the supersonic shock-wave). For High Energetic Materials (HEM), the energy release is very short, and does not need the participation of an external species. Typical high energetic materials enter the composition of explosives, pyrotechnic compositions (fireworks) and propellants (e.g. smokeless gunpowder, rocket and launcher fuels).

HEMs are used extensively both for civil engineering and military applications. There are continuous research programs to develop new materials with higher performance and enhanced insensitivity than the existing ones in order to meet the requirements of future military and space applications. Classical molecular HEMs are presented below:


TNT


RDX


TATB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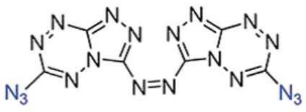
polynitrogen HEM

With the development of space propulsion, new molecular and ionic HEMs have been developed, e.g. ammonium perchlorate ($NH_4^+ClO_4^-$), ammonium dinitramide ($[NH_4]^+[N(NO_2)_2]^-$) or polynitrogen compounds, see a recent example above (J. Mater. Chem. A, 2019, 7787)

The needed HEM performance is related to heat of explosion, detonation velocity, detonation pressure, ignition delay, oxygen balance; whereas the HEM safety depends on different sensitivity types: friction, impact, shock, heat and spark. Both are important for applications.

We will present an overview of the different HEMs and their characteristics; examples of unexpected behaviors leading to explosion will be discussed, taken from open literature and our own experience. The safety rules will be emphasized to control decomposition rate and avoid explosion.

C.P. 12

Metal-Organic Frameworks (MOFs) as Prospect Adsorbents and Membranes for Energy-intensive Separations and Carbon Capture.

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Demand for functional materials targeted for specific applications is ever increasing as societal needs and demands mount with advancing technology. Evidently, improvement of existing materials and quest for new approaches to the design of novel materials are both valuable paths worth pursuing in order to address the myriad technological challenges that face us, pertaining to energy an environmental sustainability.

Metal-organic frameworks (MOFs) are a unique class of solid-state materials amenable to design and manipulation for desired function and application, thanks to advancement in reticular chemistry and the various design strategies developed for its effective practice. Several design strategies have been utilized and developed to target viable MOF platforms, from the single-metal-ion molecular building block (MBB) approach to the hierarchical supermolecular building block and supermolecular building layer approaches (SBB and SBL, respectively) to the merged nets approach, and centring structure-directing agents (c-SDA) strategy. This inherent built-in information allows access to highly stabile and made-to-order porous materials, with controlled pore-aperture size and/or inner pore system functionality, toward applications pertaining to energy and environmental sustainability. Specifically, MOF materials addressing the energy-intensive separations and carbon capture will be highlighted, as well as insights into MOF based membranes, namely pure MOF membranes and mixed matrix membranes (MMMs), construction and respective gas separation properties.

CONFERENCES

C. 1

Energy level alignment at hetero-interfaces: measurement and manipulation

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Measuring and controlling the alignment of energy bands or energy levels across hetero-interfaces is of crucial importance to steer electronic charge carriers into selected paths for a wide range of technological devices. The semiconductor industry relies on proper energy band alignment at each interface of semiconductor/high-κ/gate stacks, in order to operate transistors. Light emitting diode elements necessitate layering of several materials whose tailored band edges gradually steer electrons and hole toward recombination. Finally, controlling the alignment of molecular energy levels and energy band edges at organic/oxide interfaces, has received considerable attention for photocatalytic and photovoltaic applications.

In this paper we introduce experimental methods to measure and manipulate the energy alignment across various hetero-interfaces. Using a combination of photoemission and inverse photoemission spectroscopies, the energy alignment at metal/high-κ/semiconductor interfaces will be determined experimentally. The relationship between energy alignment across the stack and the chemical environment of each interface will be discussed. Aspects of energy alignment manipulation will be given at the organic/oxide interface. It will be shown that employing helical peptides containing strong molecular dipoles can shift the energy levels of organic layers adsorbed onto wide band gap oxides as much as 600 meV. Potential impact on device performance will be discussed.

C. 2

Nanocellulose: from hype to reality

Youssef Habibi

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In conjunction with the growing interest in developing circular economies through the substitution of fossil carbon by renewable resources, interest in biomass feedstock does not appear to wane but will continue to attract considerable attention in our society during the so-called the 4th industrial revolution.[1] In fact, with total production estimated to be 10^{13} tons with a yearly growth of ~ 3×10^{11} tons, biomass is not only abundant, renewable, and sustainable but represents the limitless potential to supplant or at minimum complement fossil resources. Therefore, the conversion of these resources into sustainable value-added chemicals, fillers, polymers, and materials is surfacing as a potential answer to face the expected scarcity of fossil resources and consequently addresses timely issues of sustainability and ecological consciousness.

Indeed, herein we argue for a renewed interest in biomass as a limitless resource of chemicals, polymers, and materials within the construct of the biorefinery for the processing, fractionation, and full recovery of all components to convert them to non-traditional high-added value and sophisticated uses. Various technologies including, but not limited to thermomechanical, enzymatic, and chemical conversions toward the production of chemicals, additives, fillers, and different classes of polymeric materials for a wide range of applications are being developed.

Since their first isolation in 1940s by Randy, nanocrystalline cellulose has started attracting the attention of the material community. Later during 1980s, Turbark group's succeeded in extracting a new kind of nanocellulose, called at that time microfibrillated cellulose, stimulating further interest in these renewable building blocks. Nowadays with the emergence of the green portfolio, numerous efforts are being focused on the use of materials from renewable resources, and we are attesting a huge and unprecedented interest in nanocellulose. This interest is due to their renewability and biodegradability, in addition to their appealing intrinsic properties such as low density, high surface area and outstanding mechanical properties. Moreover, nanocelluloses possess a spectacular ability to self-organize into liquid crystalline arrangements. All these impressive properties allow their use in a wide range of applications. This plenary lecture will provide an overview of recent advances in nanocellulose processing followed by a few examples related to their uses.

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[1] The Fourth Industrial Revolution (4IR) is the fourth major industrial era since the initial Industrial Revolution of the 18th century characterized by a fusion of technologies blurring physical, digital, and biological spheres, referred to as cyber-physical systems. It is characterized by breakthroughs in robotics, AI, nanotechnology, quantum computing, biotechnology, the Internet of Things, the Industrial Internet of Things (IIoT), decentralized consensus, fifth-generation wireless technologies (5G), additive manufacturing/3D printing and fully autonomous vehicles.

C. 3

Breaking the single-molecule detection limit using novel plasmonic nanostructures

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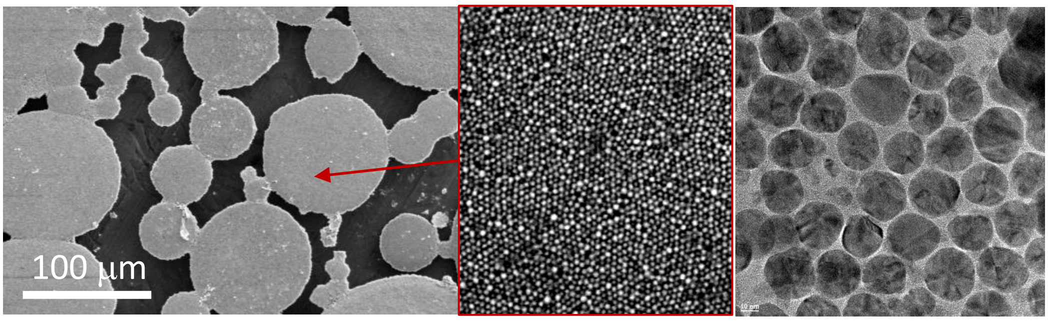
Single molecule detection was achieved by fluorescence 20 years ago and by Raman spectroscopy only 6 years later despite Raman's significantly smaller cross sections (9 to 14 orders of magnitude smaller compared to that of fluorescence). This advancement was made possible by using plasmonic nanostructures, primarily silver or gold, by the so-called single molecule surface-enhanced Raman spectroscopy (SMSERS). This extremely sensitive technique enables the detection of single vibrations which are highly influenced by various factors such as molecular interaction, charge transfer, doping elements, temperature, stress, orientation, etc. The ability to probe materials at the nanoscale is of great importance to investigate interface properties, biomolecules as proteins, pollutants, hybrid materials, and more.



Free-standing surfactant-free films (left) consisting of ~20 nm NP monolayers (center: SEM, right : TEM).

The strong enhancement involved in SMSERS results in electromagnetic and chemical effects. In the former, the nanostructure behaves as an optical nano-antenna in the visible range, while the latter, although less understood, is believed to be involved on surface electronic states resulting from the interaction of the molecule with surface defects, such as clusters of a few atoms. Our group developed a new strategy to stabilize surface defects on silver nanoparticles and to investigate the mechanism of chemical enhancement. The Raman scattering signal obtained with our nanostructures are highly intense and exhibit strong stochastic behavior. It is then possible to gain access to single-molecule reactions with an acquisition time of about only 1 ms for a full spectrum information.

This presentation will focus on the advances of enhanced Raman spectroscopy including the near-field apertureless techniques combining Raman effect and scanning probe microscopy.

Keywords: Raman, plasmonic nanostructures, single molecule detection, silver clusters

C. 4

Sustainable and advanced materials for energy: hydrogen production and batteries

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The continued exploration of advanced and sustainable materials is essential for addressing the global energy challenges. Efforts are particularly concentrated on discovering sustainable and functional materials that can be produced at scale, improving energy conversion and storage efficiencies, and integrating innovative materials into existing or new energy technologies.

In this talk, we will provide a few examples of recent developments in materials and systems for energy within our department, with a particular focus on hydrogen production and battery storage.

COMMUNICATIONS ORALES

C.O. 1

Efficient photomineralization of diclofenac using $Ce_{1-x}Zn_xO_{2-x}$ solid solution catalysts under visible light

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[2]Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé (ICPEES), CNRS University of Strasbourg, Saint-Avold Antenna, Université de Lorraine rue Victor Demange, Rue Victor Demange, 57500, Saint-Avold, France

Releases of harmful pharmaceutical compounds from industries and hospitals have harmful repercussions on the ecosystem and human health. Among the wastewater decontamination methods, heterogeneous photocatalysis emerges as an effective and promising approach for mineralizing recalcitrant organic species using light sources. Despite the good photodegradation properties of many semiconductors, poor mineralization is a common issue, primarily linked to the reactivity of O_2 with the catalyst's photogenerated electron-hole pairs. Reactive oxygen species generation relies on the molecular photocatalytic activation of O_2 through adsorption on the catalytic support. However, numerous conversions fall short due to the low mineralization capacity of polluting organic species. The formation of heterojunction interfaces in photocatalytic materials offers a solution by separating photogenerated charge carriers. In this study, we combined two oxides, ZnO and CeO_2, to develop a $Ce_{1-x}Zn_xO_{2-x}$ solid solution (called $CeZn_x$) with a fluorite structure typical of CeO_2, while ZnO exhibits a zincite structure without secondary phases. The photocatalysts prepared exhibit good efficiency against diclofenac, with ZnO and CeO_2 oxides outperforming CeZnx solid solution materials in terms of activity. However, the CeZnx materials excel in diclofenac mineralization compared to individual oxides. The most effective photo-mineralizer is found to be $Ce_{0.9}Zn_{0.1}O_{0.9}$. Oxygen-vacancy-rich $CeZn_x$-based heterojunctions were constructed to enhance oxygen chemisorption and photoexcited electron transfer. The CeZnx heterojunction system, characterized by high reactive oxygen species generation (H_2O_2, $•O_2$ and •OH), demonstrates excellent photomineralization. This research provides new insights into accelerating molecular O_2 activation and offers a practical application of photocatalysis in wastewater treatment.

C.O. 2

Synthesis and physico-chemical study of new glasses in the system Li_2O-PbO/CuO- P_2O_5

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The study of phosphate glasses has attracted many researchers for their easy preparation at low temperatures, high thermal expansion, and interesting physicochemical properties. These features make them potential candidates for various applications such as nuclear waste immobilization matrices, environmental protection, civil engineering, and biomaterials.

In this work, the phosphate glasses with general formulation $Li_2Pb_{1-x}Cu_xP_2O_7$ ($0 \leq x \leq 1$) were elaborated via the melting/quenching method. The evolution of the density and the molar volume with the composition of the synthetized glasses was investigated. The vitreous state was confirmed by both X-Ray Diffraction (XRD) and Differential Scanning Calorimetry (DSC) techniques. The thermal parameters (Tg, Tc, and the thermal stability factor) of the different glasses were determined and discussed. The obtained results revealed an increase of the glass transition temperature when the cooper content increases in the vitreous system. The nature of the different phosphate groups in the synthesized glasses was identified by Fourier Transform Infrared (FTIR) spectroscopy, and the P_2O_7 groups were identified as preponderant.

Keywords: Phosphate glasses; XRD; DSC; Thermal stability; FTIR.

C.O. 3

Electric and dielectric properties of the solid solution $Na_xCu_{2-x/2}V_2O_7$ using impedance spectroscopy

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The pyrovanadates $Na_xCu_{2-x/2}V_2O_7$ (x = 0.05, 0.1 and 0.15) were synthesized using the ceramic method, and their formation was confirmed via X-ray diffraction analysis. The X-ray diffractograms revealed that these compounds share the same crystal structure as $Cu_2V_2O_7$ [1,2]. Additionally, the presence of V_2O_7 groups was verified through infrared spectroscopy [3].To further investigate their properties, impedance spectroscopy (IS) was employed to study the electrical and dielectric characteristics in a frequency range of 1Hz to 1MHz at room temperature. The impedance spectra were analyzed using an equivalent electrical circuit model ,allowing for the determination of electrical parameters such as resistance, pseudo-capacitance, and relaxation time, as well as dielectric parameters of the pyrovanadates $Na_xCu_{2-x/2}V_2O_7$. The behavior of the alternating current conductivity (σ_{ac}) was found to follow a double power law, with its evolution at room temperature indicating a significant influence of sodium content on the conductivity properties of these compounds. Additionally, the dependence of the dielectric constant and dielectric loss tangent on the sodium content and frequency were discussed.

Keywords: pyrovanadates Copper, sodium, Impedance Spectroscopy, Electrical equivalent circuit, Conductivity (σ_{ac}), Dielectric constant

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C.O. 4

X-ray diffraction and temperature-dependent Raman scattering study of phase transitions in $Ba_{2-x}Sr_xNiMoO_6$

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The materials with double perovskite structure (AA')(MM')O_6, are solid solutions of two perovskites : AMO_3 and A'M'O_3. In (AA')(MM')O_6, A and A' represent alkaline rare earth cations (Ca^{2+}, Sr^{2+} or Ba^{2+}), while M and M' are two heterovalent transition-metal elements.

The crystallographic phase transitions as a function of temperature are common in this type of perovskite. These structural changes are often intimately related to the physical properties of materials. Because of these properties, these materials have recently attracted the interest of materials scientists [1] for possible applications in magneto-resistive devices [2] that revolutionized the computing world today. In previous studies, similar double perovskites showed other properties such as superconductivity [2], antiferromagnetic to ferri- and ferromagnetic, ferromagnetic and ferroelectric in the same phase [4], ionic conductivity [5] and catalytic properties [6], etc. Indeed, because of their important applications cited above in diverse fields, oxides with the perovskites structure in modern materials continue to grow.

In this work, we report the preparation, X-ray diffraction with Rietveld refinement and Raman spectroscopic study of phase transitions induced by composition and/or temperature in the new solid solutions $Ba_{2-x}Sr_xNiMoO_6$ (with $0 \leq x \leq 2$).

Keywords: Double perovskite, Phase transition, Raman spectroscopy, X-ray diffraction.

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C.O. 5

in-situ polymerization of intercalated 4-Vinylbenzenesulfonic Anions in NiAl layered double hydroxide nanocomposite monitored by impedance spectroscopy

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Complex impedance spectroscopy (CIS) has become a powerful nondestructive tool for investigating the properties and the quality of materials in different fields. It is based on the modeling of the obtained electrical data by an equivalent electrical circuit, which gives an insight into the physical processes that occurs inside the material.

Given its importance, studies carried out on Layered Double Hydroxides (LDH) were interested in the application of this technique and revealed that the electrical and/or dielectric behavior of LDH strongly depends on the constitution of the interlayer space (nature and arrangement of interlayer anion, water content, etc.) [1]. In the present work, the attention has been focused on using impedance spectroscopy to monitor and confirm the in-situ polymerization of the monomer Vinylbenzene sulfonate (VBS) between the layers of LDH by investigating electric and dielectric properties before and after the polymerization process.

X-ray diffraction, Fourier transform-infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy were also carried out to explore the structural properties of materials.

Keywords: Layered double hydroxide, *in-situ* polymerization, electrical equivalent circuit, complex impedance spectroscopy, Complex modulus, electrical conductivity.

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C.O. 6

In-depth study from the synthesis to the characterization of a novel glass-ceramic material breaking barriers in solid electrolyte technology

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In contrast to conventional lithium-ion batteries, which rely on liquid electrolytes, all- solid-state lithium batteries offer improved safety, longer cycle life, high energy density, and reduced requirements for the packaging and circuits used to control the state of charge. Among the diverse array of solid electrolyte options, glass ceramics, which consist of amorphous and crystalline phases, hold great promise for application in all-solid-state lithium batteries. In this respect, we have successfully fabricated a novel glass-ceramic material incorporating a newly introduced metal oxide doped phase. This was achieved by applying melt-quenching technique coupled with meticulous control over the crystallization process. Examining its crystallization kinetic has unveiled a three-dimensional nucleation mechanism accompanied by spherical particle growth with an activation energy of 165 kJ.mol^{-1}. XRD, Rietveld refinement, FT-IR, and Raman analyses verified the presence of the intended doped phase within the glass-ceramic material. Furthermore, measurements of crystallite size surrounded by glassy phase as observed from SEM images, alongside density assessments, support the formation of dense, pore-free glass-ceramic. This latter exhibits robust mechanical properties and demonstrates high ionic conductivity, achieving 1.10^{-4} (Ω^{-1}.cm^{-1}) at room temperature, while displaying low electronic conductivity of 8.10^{-9} (Ω^{-1}.cm^{-1}). This material holds promise for use as a solid electrolyte across various electrochemical devices.

Keywords: Phosphate glasses; Glass-ceramic; Solid electrolyte; Crystallization kinetic; Impedance spectroscopy.

C.O. 7

Improvement of cemented form quality of radioactive liquid organic waste using bentonite clay as addition: strength and porosity

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Radioactive waste resulting from nuclear activities must be managed safely from production to final disposal. In Morocco, the generated radioactive waste consists mainly of low and intermediate-level waste, such as liquid organic waste (LOW) [1]. Most of these radioactive wastes need to be conditioned by solidifying them in cement binder to prevent release into the biosphere. Cementation technology could enhance the effect of liquid radioactive waste by incorporating clay additives. This study aims to present a new approach to solidifying liquid organic waste, considering formulations and processes previously explored in earlier studies [2]. In the current study, the solidification of the liquid organic waste was investigated using cement binder, focusing on the improvement of the mechanical performance of the solidified waste-forms by incorporating bentonite clay. The dosage of the LOW (16 wt%, 18 wt%, and 20 wt%) of the solidified waste-forms was also probed into deeply through microstructural, mineralogical tests and compressive strength. The mechanical quality of each cemented waste form was determined by measuring it compressive strength and analyzing its porosity. The obtained results showed that the compressive strength reached more than 16 MPa after 28 days of curing, with an improvement rate of confinement of 33.33% compared to the previous studies [2] . The microstructures of the optimal waste-forms revealed that the main hydration reaction product is calcium silicate hydrate (C-S-H), which provides mechanical strength. The use of Bentonite could significantly enhance the compressive strength of solidified waste-forms and reduces the final waste volume, suggesting that it is a viable and practical addition for cementing radioactive LOW.

Keywords: Radioactive Liquid Organic Waste, Cementation Cement mortar, Solidification, Compressive strength, Porosity

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C.O. 8

Fabrication and characterization of a ceramic membrane from clay and tea waste: Application to industrial wastewater treatment

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This research demonstrates the highly effective treatment of tannery wastewater using cost-effective porous ceramic membranes, by incorporating bio-based materials, such as tea waste, as porosifying additives into the main material, which is Moroccan red clay. Various analytical techniques, including X-Ray Diffraction (XRD), X-Ray Fluorescence (XRF), Thermogravimetric Analysis (TDA-TG), Scanning Electron Microscopy (SEM), and the Archimedes principle test, were used to investigate the properties of these ceramic membranes. The impact of the pore-forming agents on the membranes physical and mechanical properties, such as open porosity, bulk density, average pore diameter, flexural and indirect tensile strength, was evaluated. Filtration tests demonstrated effective removal of turbidity, suspended matter and chemical oxygen demand from the wastewater. The optimized membrane exhibited a permeability of 1249 L/h.m^2.bar and turbidity removal efficiencies of 99.16% for tannery wastewater.

Keywords: Porous ceramic; Moroccan red clay; Tea waste; Microfiltration membrane; Tannery wastewater

C.O. 9

Sintering temperature effects on cordierite refractory ceramic derived from stevensite-rich Ghassoul clay and kaolin

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This study introduces a cost-effective approach for synthesizing refractory cordierite from a mixture of two commercially raw materials: kaolin (65 wt.%) and stevensite-rich Ghassoul (35 wt.%). The mixtures were initially milled, uniaxially compacted at 96 MPa and then sintered at 1250, 1300, 1350, and 1380°C for 1 h. The samples were characterized using X-ray diffraction (XRD), differential thermal/thermogravimetric analysis (DTA/TGA), scanning electron microscopy (SEM), dilatometry, three-point bending and diametral compression tests. The DTA results indicated that cordierite crystallization occurred at a temperature of 1240°C. The Rietveld quantitative phase analysis revealed a continuous increase in the proportion of cordierite phase from 94.4 wt.% at 1250°C to 99.8 wt.% at 1380°C. Mechanical properties exhibited an improvement with increasing sintering temperature, and cordierite sintered at 1380°C revealed optimal performance: flexural strength of 44.4± 4.6 MPa, tensile strength of 20.2±2.5 MPa, and Young's modulus of 34.6±2.4 GPa. The coefficient of thermal expansion (CTE) for cordierite sintered at 1380°C was 2.96□10-6 °C^{-1}.

Keywords: cordierite, stevensite, Ghassoul, refractory materials, mechanical properties.

C.O. 10

Comparative experimental massifs of different roller-compacted concrete compositions intended for dam construction

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Roller-compacted concrete (RCC) dams are massive structures that require the placement of large volumes of concrete and must meet precise quality standards.

To ensure their construction under optimal conditions and quality, we conducted the creation of experimental massifs, also known as test panels, with the main objectives of refining the general implementation process and verifying the in-situ characteristics of RCC. For each experimental massif, we adopted a volume of 2000 m^3 of RCC, constructed in 7 layers of 30 cm of thickness, with different formulations expressed as F/S/C, representing Filler (fines), Sand 0/4mm, and Cement dosage, respectively.

Following various in situ tests and measurements (density, water content, porosity, compressive and tensile strength, lugeon tests, etc.), the results allow us to distinguish two formulations suitable for adoption in the body of the dam.

Keywords: Roller-compacted concrete, experimental massif, porosity, density, strength

C.O. 11

Reactivity of red clays with hydraulic lime in the presence of phosphogypsum and steel slag

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Red clay, a mineral formed from various rocks in the Earth's crust under humid and hot climate conditions, exhibits accelerated disintegration [1-2]. Despite its high-water content, high void ratio and high plasticity, high bearing capacity, low compressibility and good mechanical properties, read clay is filling material for building foundations bearing layers [1]. The traditional method of enhancing the mechanical properties of clays involves stabilizing them with lime [3]. Industrial by-products such as phosphogypsum (PG) and black steelworks slag (SC), can be integrated into red clay-rich soils. This study aims to assess the impact of PG and SC on lime-stabilized red clay .. Geotechnical, physico-chemical and mineralogical characterization of red clay and lime-PG-SC mixtures was carried out using a varioustechniques, including X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR-IR), thermal analysis (DTA-TG), scanning electron microscopy (SEM), Atterberg limits and sedimentometry.

Red clay is composed of quartz, illite and hematite, with 19.7% organic matter, classified as clay loam with 42% clay, 48% silt and 10% sand. The addition of lime, PG and SC modifies the physicochemical parameters of the clay and reduces the plasticity index of the clay. Compressive strength improves after 28 days of curing, for mixtures with 32% lime. This strength increase results from short-term changes in structure and mineralogy, coupled with increase long term cohesion enhancement .Lime raises the pH, destabilizing the clay structure, with released aluminates and silicates reacting with calcium to form the Calcium-Silicate-Hydrate (C-S-A-H) cemented gel. The presence of PG allows ettringite formation. The combined addition of PG and SC improves the mechanical properties of lime-stabilized red clays.

Keywords: Red clay, Phosphogypsum, Steel slag, Stabilisation, uniaxial compression

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C. O. 12

Herbicide detoxification from synthetic effluents using Moroccan organophilic clay: A comparative study

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The present study focuses on the adsorption of a toxic herbicide onto Moroccan organophilic clay using two distinct methods: a single-stage method, where organophilization and adsorption occur simultaneously [1], and a two-stage method, where organophilization and adsorption are carried out separately. The results obtained demonstrate a superior efficiency of single-stage adsorption compared to two-stage adsorption. Additionally, this study allowed us to evaluate the impact of herbicide concentration, intercalary cationic surfactant percentage, and residence time on the adsorption process [2]. These findings underscore the importance of considering not only adsorption methods but also environmental parameters and properties of adsorbent materials in the development of effective strategies for pollution control and treatment of contaminated water [3].

Keywords: adsorption process; toxic herbicide; cationic surfactant; Moroccan organophilic clay.

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C. O. 13

Optimization of sugar industry waste for microfiltration membrane based on clays in textile industry wastewater treatment

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It is the responsibility of the scientific community to devise innovative, cost-effective, and environmentally friendly membrane materials for tackling the treatment of industrial wastewater. The present work reports the development characterization of a low-cost microfiltration ceramic membrane crafted from natural Moroccan clay and sugar scum. Utilizing the Doehlert design-based Response Surface Methodology, we optimized preparation conditions, specifically focusing on the impact of sugar scum quantity, sintering temperature, and sintering time on mechanical strength, water absorption, and porosity. The optimized membrane has compressive strength of 56.1 MPa, a water absorption of 26.3 %, and a porosity of 42.7 %, a water permeability of 1250 L/ h.m^2.bar, a 0.9 µm of average pore size and excellent chemical corrosion resistance in basic media. Evaluating the optimal membrane's performance through frontal microfiltration of industrial wastewater revealed impressive removal rates, with 99% for turbidity and 63% for chemical oxygen demand (COD).

Keywords: Ceramic membrane; Microfiltration; Optimization; Response surface methodology

C.O. 14

Thermal transport and chemical properties of phosphogypsum and steel slag add to the bentonite-lime mixture

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Morocco's phosphate industry generates over 15Mt per year of phosphogypsum (PG), which is often dumped into the sea, leading to significant environmental and health hazards. This study aims to valorize by incorporating it into a clay-lime mixture for road construction purposes. Additionally, steel slag, a by-product of the steel industry in Morocco, was added to improve the mechanical properties of the clay-based material.

Chemical and mineralogical compositions of the raw materials were analyzed using X-ray diffraction (XRD) and X-ray fluorescence (XRF). XRD results show that bentonite is predominantly composed of calcium and sodium montmorillonite, lime is composed of calcium hydroxide, periclase and calcite. PG is composed of gypsum, and slag contains calcium silicate, calcium iron oxide, metallic iron and quartz. XRD of the bentonite-lime (BL) mixture showed the formation of a calcium-silicate-hydrate (C-S-H) gel on montmorillonite surface. The addition of PG to the (BL) mixture, hydrated sample (BLPG), allows the formation of the C-S-H gel and ettringite. The addition of slag to the (BLPG) mixture, hydrated specimen (BLPGSs), does not allow the formation of new phases.

The study further investigated the evolution of permeability coefficients over time for bentonite, BL, BLPG, BLPGSs specimens. Permeability coefficients is almost constant of bentonite but exhibited two distinct stages for BL, BLPG, and BLPGSs specimens, with an initial rapid increase at 0-21 days followed by a slower saturation stage, resulting in enhanced impermeability after 101 days. Thermal transport properties, including thermal conductivity, thermal diffusivity, thermal effusivity and volumetric heat capacity of bentonite and BL, BLPG and BLPGSs specimens were also examined, indicating a decrease in all of these parameters with the addition of lime, PG, and steel slag to bentonite. Furthermore, as the proportion of bentonite decreased, thermal transport properties decreased.

Keywords: Bentonite, Thermal transport properties, Permeability, Lime, Phosphogypsum, Steel slag.

C.O. 15

Physico-chemical and mechanical characterization of a phosphogypsum based road material

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The transformation of phosphate ore into phosphoric acid entails the generation of phosphogypsum, one of the most remarkable solid by-products in Morocco, the output of which is about 30 million tons per annum. It is an acid residue that contains, in addition to gypsum, impurities that accompanied the phosphate rock, including heavy metals and radionuclides which cause serious environmental impacts. From a mechanical point of view, phosphogypsum is a weak material, yet it is its acidic nature that hinders its use as a road material, since it increases its solubility which in turn makes it sensitive to water variations. A new approach is proposed to valorize phosphogypsum, through the correction of its acidity, for a massive utilization in road engineering, while taking into account technical, economic and environmental constraints. Lime-activated fly ash was chosen as the stabilizing material. Thus, mixtures of phosphogypsum, fly ash and quicklime were developed in order to evaluate the effect of the treatment on the physico-chemical and mechanical behaviour of phosphogypsum. To this end, compaction tests, unconfined compressive strength (UCS) tests, X-ray diffraction (XRD) analyses, thermal analyses (TGA/DTA) and scanning electron microscope (SEM) observations were performed on the mixtures at 28 days of curing. The results showed an increase in mechanical strength with the increase in fly ash and lime content which was explained by a densification of the matrix following the pozzolanic reaction at the origin of the formation of new binding mineral phases.

Keywords: Valorization, Phosphogypsum, Fly ash, Lime, Road material, pH, Pozzolanic reaction.

C.O. 16

Synthesis and structural study of new phosphates: $MMg_2Fe(PO_4)_3$ (M = Ba, Sr) with the α-$CrPO_4$ type structure

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The orthophosphates with α-$CrPO_4$ type have a great interest, related to their structural type, generating interesting physico-chemical properties.

In this paper, we report the synthesis and the structural study of the two new phosphates $MMg_2Fe(PO_4)_3$ (M = Ba, Sr). The crystal structures of the two compounds were solved in the orthorhombic system, space group Imma, using single crystal XRD data. This symmetry belongs to α-$CrPO_4$ type structures mentioned in the literature **[1]**. The structure of the both compounds is building up of MgO_6 octahedra, FeO_6 octahedra and PO_4 tetrahedra. The connection between those polyhedra leads to a threedimensional network delimiting hexagonal tunnels which are occupied by Ba and Sr cations.

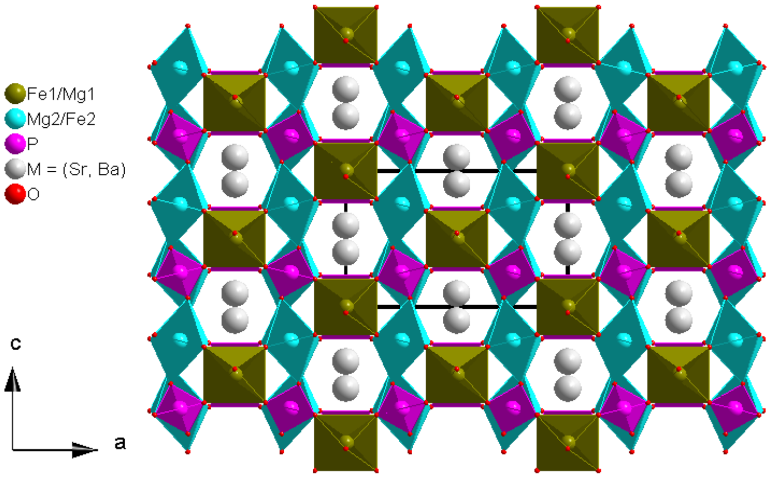

Figure 1 : Representation of the crystal structure of $MMg_2Fe(PO_4)_3$ (M = Ba, Sr)

Keywords: Phosphate, α- $CrPO_4$, DRX, single crystal.

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C.O. 17

Comparative study of low-grade phosphate tailings beneficiation via organic acid leaching and reverse flotation

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This study investigates the beneficiation of rejected phosphate-washing sludge (Ps) using different techniques. We compared the acid leaching method with attrition scrubbing and desliming followed by reverse flotation. The analysis showed that acetic acid was the most effective leaching agent and the optimum leaching parameters were 7% acetic acid concentration, 30% solid concentration, 100 min reaction time, and 40 ◦C temperature. We also found that the flotation time and pulp pH have the most significant influence on P_2O_5 grade and recovery, followed by ester dosage, while amine dosage was the less significant parameter. The optimum flotation conditions were 10 min flotation time, 481.81 g/T ester dosage, 400 g/T amine dosage, and 4.58 pulp pH. These optimum conditions yielded a P_2O_5 grade of 28.61% and a recovery of 71.5%. This study provides valuable insights into choosing the best technique for enriching Ps for various applications.

Keywords: Phosphate-washing sludge; Beneficiation; Organic acid leaching; Reverse flotation, Design of experiment; Optimization.

C.O. 18

Phosphate washing-sludge Contamination: undesirable elements and environmental issues

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Morocco's enormous quantities of phosphates and their vital economic importance in the country's development fully involve the necessity of systematic research in this area.

The phosphate processing industry produces large quantities of "waste", mainly discharged into the sea. Phosphate processing industry produces large amounts of "waste", mainly discarded at sea. During the process, that contains the washing treatment to remove undesired minerals, the phosphate sludge was stored for several months. However, this sludge can introduce undesirable elements such as heavy metals (U, Mn, Cd, As, V, Cr, Zn, Cu, Ni, etc.), organic pollutants and pathogenic germs, the flow of which must be controlled to ensure environmental safety. As a result, heavy metals can enter the food chain through food consumption, raising concerns about their potential impact on human health. There are worries over the possible effects of heavy metals on human health because they can enter into the agriculture products. In this regard, before the exportation of agricultural produce, the concentration of heavy metals is monitored which should adhere to the standers.

This work brings about three points. First, systematic review sheds light on the effects phosphate washing-sludge on soil. The second point involves characterizing muds to determine their chemical elements. Third, an experience approach that may be used to overcome the phosphate washing-sludge issue will be presented.

Keywords: Phosphate washing sludge, pollutants, environment.

C. O. 19

Decomposition of phosphogypsum into CaF_2 and $Li_2SO_4.H_2O$ by mild process

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Phosphogypsum (PG) is an acidic byproduct resulting from phosphoric acid production, typically stored or discharged into water surfaces, causing various environmental pollution issues. The objective of this study is to lessen this environmental risk by converting PG into calcium fluoride (CaF_2) and lithium sulfate hydrate ($Li_2SO_4.H_2O$), two highly useful practical products through a reaction with lithium fluoride. The parameters examined to optimize reaction conditions include the initial concentration of reactants and reaction time.

Furthermore, the formed products were primarily characterized using several characterization techniques, including chemical analysis by ICP, structural analysis by X-ray diffraction and Fourier-transform spectroscopy, thermal analysis by TGA-DTA, and morphological analysis by SEM-EDX. The results reveal that the predominant factors influencing the decomposition process are the initial concentration of reactants and the reaction time. The optimal efficiencies are 94.3% for CaF2 and 96.59% for $Li_2SO_4.H_2O$ during the conversion of PG.

Keywords: phosphogypsum, lithium fluoride, calcium fluoride, lithium sulfate.

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C.O. 20

Matériau naturel pour le traitement de l'acide phosphorique industriel : Caractérisation stratigraphique, minéralogique & géochimique

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Le présent travail s'inscrit dans le cadre d'un projet Recherche/Développement autour des phosphates sur le Traitement de l'acide phosphorique industriel par un matériau naturel. Il a pour objectifs, la réalisation d'une étude géologique dans la région des Doukkala afin de caractériser, localiser et évaluer les gisements exploitables.

La zone du Sahel-Doukkala comporte des séries sédimentaires allant du Paléozoïque au Miocène, sur lesquelles reposent des dépôts transgressifs plio-quaternaires. Les terrains éocènes, célèbres par leurs gisements de phosphates sont absents dans cette région. Le Crétacé est extrêmement important dans la région et constitue le substratum presque continu des terrains plio-quaternaires. Le Cénomanien, composé de roches carbonatées, s'étale sur toute la région entre le Cap d'El Jadida et l'embouchure de l'Oued Oum Rbia.

Afin d'étudier ces formations, nous avons échantillonné de manière relativement systématique dans deux zones : Ain Talmest et Jorf Lasfar dans la région d'El Jadida. Leur caractérisation stratigraphique, pétrographique et géochimique est une étape fondamentale pour leur éventuelle valorisation. L'étude litho-stratigraphique réalisée en exploitant 19 sondages dans la région, montre qu'on plus de la variation lithologique, nous assistons à une évolution d'épaisseur qui varie de 7 m à l'Est et qui peux atteindre 100 m vers l'Ouest avec un volume total estimé à 103 km^3, pour une superficie de 2033 km^2.

Les résultats obtenus à partir de l'analyse microscopique des échantillons prélevés, montrent une dominance des carbonates caractérisés généralement par des microfaciès dolomitiques avec des textures wackestone à mudstone. Ces échantillons sont formés principalement de deux fractions : une fraction grossière (90%) contenant de la dolomite et du quartz, et une fraction argileuse (10%). La caractérisation géochimique par Diffraction des rayons X (DRX), montre que ces échantillons sont formés principalement de dolomite, de quartz et d'argile de type illite et parfois kaolinite. L'utilisation du Microscope électronique à balayage couplé à la spectrométrie à dispersion d'énergie (MEB-EDX) a montré que le minéral dominant de ces roches est la dolomite dont la taille est comprise entre 3 et 30 µm. La cartographie chimique montre une composition par les éléments Si, Al et Fe, indiquant la présence de quartz et d'argile. L'analyse pondérale des échantillons, par fluorescence X, donne une composition riche en Mg (40%) et Ca (32%) ce qui confirme le caractère dolomitique de ces roches. On note aussi la présence de Si (12%) et d'Al (10%), indiquant l'existence de quartz et d'argile, avec un peu de Fe (1,8%).

Mots clés : *Carbonates, Cénomanien, Stratigraphie, pétrographie, géochimie, Sahel-Doukkala, Maroc*

C. O. 21

Crystalline and vitreous $Na_{3.89}Ca_{0.67}Fe_{0.23}Ti_{0.77}(PO_4)_3$ Synthesis, structure, physico-chemical and spectroscopic characterizations

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Titanium phosphates materials in both crystalline and glassy forms have been studied for their various applications, such as batteries [1], nonlinear optics [2], biomaterials [3], etc,.. In this work, $Na_{3.89}Ca_{0.67}Fe_{0.23}Ti_{0.77}(PO_4)_3$ phosphate in vitreous and crystalline forms was prepared and structurally characterized by XRD, DTA, density, Raman, infrared, uv-visible, and magnetic measurements. The crystalline compound belongs to the Nasicon family. Its structure was determined at room temperature, from powder X-ray diffraction data using the Rietveld method, in R32 non-centrosymmetric space group. It consists of a 3D network of PO_4 tetrahedra and AO_6 (A = Na/Ca, Fe/Ti) octahedra sharing corners. One of the two positions of the octahedral sites is statistically occupied by Na^+ and Ca^{2+}, the other position is statistically occupied by Fe^{3+} and Ti^{4+}. The remaining sodium ions occupy interstitial sites usually labelled M1 and M2. The detailed crystallographic formula is $[Na]_{M1}[Na_{2.56}]_{M2}[(Na_{0.33}Ca_{0.67})(Fe_{0.23}Ti_{0.77})]_A(PO_4)_3$. Comparison of Raman, infrared and uv-visible spectra, and magnetic measurements of glassy and crystalline forms of the studied phosphate allowed us to obtain some information on the structure of the glass.

Keywords: Titanium iron phosphate; Nasicon; Glass; Structural characterization; Magnetic properties.

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C. O. 22

Study of the retention of Fe^{2+} by dicalcium phosphate dihydrate

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Recent work carried out in our laboratory shows that dicalcium phosphate dihydrate, $CaHPO_4\ 2H_2O$ (DCPD), exposed to solutions of nickel or copper ions, manages to immobilize these metal ions by ensuring their conversion into insoluble phases of $Ni_3(PO_4)_2$ or Cu_2PO_4OH. In addition to proving the ability of the DCPD to remove metal ions from aqueous solutions, this work establishes undemanding methods for the preparation of nickel and copper phosphates that are highly coveted due to their optical, magnetic, and catalytic properties. Given the reactivity of this calcium phosphate towards nickel and copper, we can expect similar performances with respect to iron. The possibility of preparing a new iron phosphate by a method similar to that established for nickel phosphate and copper hydroxyphosphate could open up new perspectives for the use of dicalcium phosphate. This article focuses on the study of the retention of Fe^{2+} by DCPD. It describes the changes observed in solutions and solids when the same amount of DCPD is introduced into Fe^{2+} solutions of different concentrations. It also provides information on the mechanisms involved in the modifications that phosphate and solutions undergo during exposure. Among the main changes that will be presented, the clear decrease in iron content and the clear increase in calcium content detected in all solutions following their exposure to phosphate. As an indication, for an iron solution initially prepared such that the number of moles of Fe^{2+} in solution is the same as that of Ca^{2+} in the solid, the yield of iron removed from the solution and the yield of calcium released by the phosphate reach 97%. Such changes obviously cannot occur without consequences on the solid phosphate. As will be described, inductively coupled plasma mass spectrometry, X-ray photoelectron spectroscopy, and scanning electron microscopy applied to solids reveal that, upon exposure to these solutions, DCPD loses its calcium ions and incorporates iron ions. Depending on the concentrations of the iron solutions and the exposure time, X-ray diffraction and infrared spectroscopy show that the exchange between calcium and iron that DCPD undergoes occurs without change in structure or gives rise to a metal phosphate consisting mainly of an amorphous phase.

C.O. 23

Modeling and Optimization of the Industrial Phosphoric Acid Pretreatment Process by Natural Calcite: From Laboratory to Industry

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Industrial phosphoric acid, obtained through the acid attack of phosphate rock, inevitably contains undesirable impurities such as sulfate, fluoride, organic matter, and metals. These impurities impact process selection, production equipment, production costs, and the environment, necessitating pretreatment of the produced acid for use in fertilizer production, sale to individual customers, or purification treatment.

Building on previous work [1,2], a natural material based on calcite is employed for the pretreatment of industrial phosphoric acid. Physico-chemical characterization (XRD, XRF, FTIR, and SEM) and geological studies have revealed that this material is primarily composed of calcite with a low magnesium content, which poses detrimental issues for the production of phosphoric acid and its derivatives. Additionally, a small fraction of illite-type clay and quartz is present. This material has demonstrated efficacy in improving the quality of industrial phosphoric acid by retaining impurities (sulfate ions, fluoride, organic matter, heavymetals, etc.) using a simple protocol that can be integrated at an industrial scale. The semi- pilot station, designed at the laboratory level as part of the R&D project on phosphates "APPHOS-ID: TRT-ZAK-01/2017," facilitated the adjustment of several factors related to thecontinuous regime of the pretreatment process. Optimization of operating conditions is achieved through modeling with a full two-level factorial design strategy with three factors (quantity of natural material, temperature, and pretreatment time), taking into account conditions available at the industrial site and ensuring a Ca/SO_4 molar ratio equal to 1 in the pretreated phosphoric acid.

Exploration of the obtained results demonstrated the dual benefit of treating 29% P_2O_5 phosphoric acid with this material. It reduces concentrator downtime by more than 50% and allows the elimination of the pretreatment step for 54% P_2O_5 phosphoric acid using the currently employed natural phosphate. In addition, there is a financial profitability (Gain/Cost) of 2.39. For a potential transfer to the industry, a monetary estimate is established to conduct trials on an industrial scale.

Keywords: Phosphoric acid, Natural material, valorization, optimization, technological transfer.

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C. O. 24

Valorization of Moroccan phosphate wastes: physico-chemical characterization and application for phosphoric acid desulphation

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Prioritizing the exploitation of low-grade phosphate ores and phosphate mining waste rock has become crucial due to the increasing demand for phosphate, particularly for the fertilizer industry. Accordingly, further beneficiation is required to achieve market requirements.

During the beneficiation process, sedimentary phosphate is separated from associated gangue minerals like clay, limestone, and silicates through various steps such as crushing, screening, washing, and flotation. These operations produce significant waste, comprising phosphate sludge and waste rock, typically stored at the mining site [1]. This study aims to evaluate the potential of two types of phosphate: phosphate beneficiation waste and low-grade phosphate for the desulphation of industrial phosphoric acid.

Phosphate samples from the Khouribga mining site in Morocco were analyzed using XRD, XRF, ICP-AES, FTIR, TGA-TDA. Phosphate beneficiation waste reveals the presence of minerals like calcite, dolomite, quartz, and fluorapatite. The chemical composition includes significant proportions of CaO (49%), P_2O_5 (11%), and SiO_2 (7%). Moreover, low-grade phosphate primarily consists of calcite and fluorapatite, with notable concentrations of CaO (53%), and P_2O_5 (14%). In both samples, different bonds and groups (P–O, CO_3^{2-}) were highlighted by FTIR analysis, whereas TGA-TDA indicated the decomposition of carbonate.

The low grade is used directly to desulphate phosphoric acid 29% P_2O_5, while the waste required a simple treatment. The process used is simple, operating under industrial-scale conditions. The results obtained indicate that both types of phosphate present a significant source of calcite and phosphorus. For phosphoric acid desulphation, low-grade phosphate ore and beneficiation phosphate waste improve the quality of phosphoric acid while preserving the P_2O_5 content of the desulphated acid.

This study highlights the importance of exploiting low-grade phosphate ore and phosphate beneficiation waste to improve the quality of phosphoric acid and provide a more efficient and sustainable solution for the phosphate industry.

Keywords: Beneficiation phosphate waste, Low-grade phosphate, Valorization, Phosphoric acid, Desulphation.

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C.O. 25

Investigating the Influence of Polysaccharide on the Physical and Chemical Properties of Carbonated Apatite Bone Cement

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Calcium phosphate cements (CPCs) are extensively used as synthetic bone grafts to repair bone defects due to their advantageous properties including natural bone-like composition, excellent biocompatibility, bioactivity, and osteoconductivity [1]. The ability of CPCs to harden *in vivo* at low temperature and their intrinsic porosity are the main advantages of CPCs, allowing the incorporation of various bioactive molecules, and making them excellent candidates for drug delivery applications [2]. However, the clinical application of CPCs is hampered by their poor rheological properties and brittle mechanical behavior. Furthermore, bone infection pathologies remained a challenge in bone regeneration. In this light, the current study aims to develop a composite cement (CaP-$CaCO_3$-PS-ATB) based on calcium phosphate (CaP), calcium carbonate ($CaCO_3$), polysaccharide (PS), and an antibiotic (ATB) for bone regeneration and treatment of bone infections.

The effect of PS and ATB on the physicochemical and rheological properties (cohesion, injectability, and compressive strength) was investigated. Furthermore, the *in vitro* release of the ATB through the composite matrix as well as the antibacterial activity were investigated. FTIR and XRD characterization revealed that the setting reaction of the prepared composites leads to the formation of a nanocrystalline carbonated apatite, similar to bone mineral. The evolution of cement characteristics stated that combining CaP-$CaCO_3$ cement with the polysaccharide and the antibiotic is an interesting strategy for the development of composites with improved mechanical, setting, and rheological properties allowing their use in minimally invasive surgical techniques. Drug release tests revealed prolonged and controlled profiles over several days. Moreover, antibacterial activity tests showed that the amounts released per day are sufficient to inhibit staphylococcus aureus the strain responsible for bone infections.

The findings indicated that the developed composite cements could be promising candidates for substitution and localized treatment of bone infections.

Keywords: Calcium Phosphate cement, polysaccharide, physicochemical properties, mechanical properties, antibiotic release

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C.O. 26

Development of Calcium Phosphate Cement for Therapeutic Use: Formulation, Physicochemical Properties, and Release Study

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Calcium phosphate cements (CPCs) are promising substitute materials for bone-related defects in biomedical fields, due to their outstanding biocompatibility, biodegradability, and osteoconductivity. In addition, the setting at low temperatures makes these materials promising carriers of different types of drugs, such as antibiotics, analgesics, anti-cancer, anti-inflammatory, as well as growth factors [1]. This study aims to develop CPC composites loaded with an antibiotic for drug delivery application. The characterization, using various and complementary techniques, and the antibiotic release behaviors were investigated.

Two different groups of composites were formulated. (i) In the first group, the antibiotic was loaded into the calcium phosphate cement (CPC-ATB). The second group consists of incorporating the antibiotic into a polymer (PM) based composite cement (CPC-PM-ATB). The physicochemical characteristics of the prepared materials were performed. The obtained results showed that the antibiotic-loaded composites were successfully formulated. In addition, the presence of the ATB antibiotic in the composites' matrix did not affect the structure of the composites.

The drug release behaviors were evaluated over 10 days in terms of the ATB amount released per day. The results indicated a massive release of the ATB during the first day (25-40 mg. L^{-1}), and then stabilized and remained constant (0.5-8mg.L^{-1}/ day) for the rest of the test period. Furthermore, the release behavior was affected by the association with the PM revealing a remarkable decrease of elution rate. Finally, the modeling antibiotic release kinetics with several models indicated that the ATB release was controlled by a diffusion mechanism. The released doses are largely sufficient to inhibit virtually all staphylococcal strains and methicillin-resistant Staphylococcus aureus.

The obtained results on the formulated composites make them promising materials as a local antibiotic delivery bone-substitute material, especially for the prevention of bone-implant-associated infections.

Keywords: Antibiotic, Calcium Phosphate, Cement, Composite, Drug delivery system, Polymer.

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C.O. 27

Eco-friendly wastewater treatment using a crab shell-based liquid bio- F coagulant: Multi-criteria decision analysis related to different pollutants Separation

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The protein-rich liquid resulting from the deproteinization step of the chitin /chitosan production process is proposed as a novel wastewater bio-coagulant. The raw material for producing the bio-coagulant is the crab shell contained in discarded fishery by-products. The protein content of the liquid, determined by OPA assay, was 31.6 mg/L. FT IR spectra proved the presence of chitin, and SEM images showed the presence of a nanoparticulated chito-protein complex in the liquid. Coagulation tests were performed with fisheries wastewater, in which the influence of different parameters, such as the bio-coagulant dose, the pH, the agitation speed, and the settling time, on the effectiveness of the bio-coagulant were investigated. Since different parameters with values in wide ranges may affect the fisheries wastewater treatment by the use of the new liquid bio-coagulant, a multicriterial optimization analysis based on Box-Behnken and response surface method (RSM) was applied. The optimal removal degrees, in terms of turbidity (98.91 %), BOD_5 (92.05 %), and COD (78. 92 %) were achieved at a bio-coagulant dosage of 17.5 ml L of fish processing wastewater (FPW) at pH 11.3 and temperature of 25 °C. A good fit resulted from the experimental data, the Box-Behnken regression models, and response surface-calculated data. The results revealed new bio-coagulant effectiveness similar or superior to the commonly used chemical coagulants (ferric chloride, aluminum sulfate) and even to commercial chitosan. The obtained data indicate that the new natural liquid bio-coagulant is environmentally friendly and suitablefor fisheries wastewater treatment.

Keywords: Crab shell, Chito-protein, Bio-coagulation, Fish by-product, Fisheries wastewater, Box-Behnken.

C.O. 28

A Critical Review of the Enhanced Recovery of Rare Earth Elements from products and waste products of phosphate industry

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Rare earth elements (REE) is a term that corresponds to 17 chemically similar metallic elements (15 lanthanides plus scandium and yttrium). Thanks to their unique properties, their application has gone beyond the classical use as basic materials in many technologically advanced products (satellite, automotive, defense ...). Today, they are becoming increasingly important in the transition to a low-carbon circular economy, given their essential role in permanent magnets, lamp phosphors, rechargeable nickel-metal hydride batteries, catalysts and other green economy applications. As a result, the demand for REE has grown significantly, from 75,500 tonnes of rare earth oxides (REO) in 2000 to 123,100 tonnes of REO in 2016. Moreover, the European Commission considers rare earths as the most critical group of raw materials with the highest supply risk. Thus, the recovery of these strategic elements from secondary sources is a mandatory option. Bastnasite, monazite and xenotime are the three most frequently mined rare earth minerals (primary sources of REE) .The lack of an economically viable and operational primary deposit is driving many countries (as Morocco) towards the exploitation of secondary sources such as end-of-life products (permanent magnets, fluorescent lamps, nickel-metal hydride batteries). In parallel, researchers are obliged to test the REE recovery potential from other likely secondary sources such as apatite and gadolinite. A large number of REE-bearing phosphate minerals have been found in nature, this indicate that REEs have a strong affinity towards phosphates. In this regard, our study summarized and classified various enhanced methods for the recovery of REEs from products and waste products of phosphate industry. The advantages and disadvantages of various methods were compared and an optimal possibility of a phosphate circular economy was suggested.

Keywords: Rare earth elements- phosphate -circular economy- recovery - waste products.

C.O. 29

Elaboration of geopolymer concrete using seawater and sand-waste material: synthesis, microstructure, and mechanical behavior

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Recently, the availability of river sand has declined, posing challenges for many countries to satisfy their construction needs. Utilizing sea sand for construction has emerged as a solution to address the scarcity of river sand. This research aims to assess the properties of geopolymer paste derived from seawater and sea sand, which have gained popularity due to their abundance, cost-effectiveness, and environmental benefits. The investigation involved creating various geopolymer mixtures by adjusting the ratios of seawater, sea sand, and alkaline activators. Results indicate that the geopolymer's compressive strength increased as curing time progressed, with seawater and sea sand playing a significant role in enhancing strength development. Furthermore, incorporating sea sand improved workability and reduced water requirements. Consequently, this study concludes that incorporating seawater and sea sand into geopolymer production offers a sustainable substitute for traditional concrete materials.

Keywords: Geopolymer, Seawater, Sea-sand, Concrete and mortar, Compressive strength

C. O. 30

1-D copper(II) coordination polymer based on 2,5-bis(pyridine-2-yl)-1,3,4-thiadiazole as bridging ligand: Synthesis, structural characterisations, Hirshfeld surface analysis, and biological assessment

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In recent years, heterocyclic ligands have garnered significant attention within the realm of materials science, particularly in the domain of coordination chemistry. This heightened interest can be attributed to their remarkably versatile coordination modes, leading to a wide array of structural possibilities. These ligands have demonstrated their capacity to engender monomers, dimers, and even coordination polymers when combined with transition metals like copper (II), nickel (II), and cobalt (II). Such an approach finds applications in various fields such as biology, catalysis, and the pharmaceutical industry **[1].** Of late, the utilization of 1,3,4-oxadiazole and 1,3,4-thiadiazole moieties has yielded mono- and bimetallic complexes, as well as coordination polymers with magnetic and biological properties **[2,3].**

In this work, a new copper (II) mono-dimensional coordination polymer based on 2,5-bis(pyridine-2-yl)-1,3,4-thiadiazole (*bpt*) as bridging ligand, noted $[Cu(bpt)Cl_2]_n$, has been synthesized by reaction of L with copper salt ($CuCl_2 \cdot 2H_2O$) and characterized by single crystal X-ray diffraction, UV-Visible, and FTIR techniques, as well as Hirshfeld surface analysis. This new 1-D Cu^{II} coordination polymer exhibited elevated antimicrobial activity against several strains of the fungal phytopathogens *Verticillium dahliae* and *Fusarium oxysporum* fsp. *melonis* suggesting its use as a fungicide in crop protection.

Keywords: 2,5-Bis(pyridin-2-yl)-1,3,4-thiadiazole; 1-D CuII complex; Crystal structure; Coordination chemistry; Antifungal activity.

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C.O. 31

Development and characterization of innovative, active and intelligent packaging films

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Colorimetric films were developed using cellulose acetate (CA) as a base matrix in the presence of red cabbage anthocyanins (ANT) as a natural colorant and thymol as an active agent. CA/THY/ANT films with different concentrations of ANT were prepared using the solvent evaporation method, to control food freshness and improve shelf life. The prepared films were characterized by FTIR, SEM and other techniques. Anthocyanin-rich red cabbage extract confers to the films a clear, stable and reversible color response in a pH range between 2 and 12, and average antioxidant properties. Thymol was added to the label as natural food preservative. The antibacterial properties against the pathogens tested were improved, without affecting the clear coloration of the films and their response. To validate the use of these films as an indicator of food freshness, application tests were carried out on various food types. The films showed improved sensitivity to pH changes and a beneficial effect on the acidity and color of foods during storage. The films also revealed a reduction in bacterial load in foods during storage at different temperatures and a possibility of reuse, by regeneration of the initial color. These results confirm the possibility of using these new smart films to control freshness and extend the shelf life of foods.

Keywords: Cellulose acetate, Food preservation, films, packaging.

C.O. 32

Behavioral studies of Phosphate Sludge-Incorporated Geopolymer Concrete Submitted to Elevated Temperatures

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Geopolymer concretes have been increasingly used as a suitable alternative in industrial sector. However, if geopolymer concrete is mixed using a single feedstock, its performance is often severely limited by the physical/chemical characteristics of the feedstock. Thus, it is judicious to integrate feedstocks derived from industrial solid wastes to elaborate geopolymer concrete. In this study, untreated phosphate sludge (UPS) and Metakaolin (MK) were used to prepare sodium and/or potassium-activated unitary and binary geopolymer concretes and the microstructure, physical properties, and high-temperature performance were systematically investigated. The results showed that incorporating 50% of UPS significantly enhances the mechanical properties of geopolymer concretes with a 28-day compressive strength reaching 5.49 MPa. After treatment at 800°C, the elaborated concrete transformed from amorphous and semi-crystalline gel structures to a crystalline structure, regardless of the mix designs. Geopolymers activated with mixed alkali metals (Na/K) showed thermal shrinkage features, enabling structural compaction with minimal density loss, which is beneficial for their mechanical properties below 500°C. The abundant CaO in the UPS acts as a self-fluxing component to decrease the sintering temperature during geopolymer fritting, thus reducing temperatures that cause unexpected stiffness loss.

Keywords: Binary geopolymer concrete; Untreated phosphate sludge; High temperature; Mechanical properties

C.O. 33

The influence of a newly developed phosphonate derivative on the corrosion resistance of carbon steel in a 1N H_2SO_4 environment

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In industrial settings, acidic solutions are commonly used, raising concerns about the corrosion of steel in such environments. Sulfuric acid, widely employed for tasks like cleaning, pickling, descaling, and acidizing, poses a significant threat to iron and its alloys due to its corrosive nature. To mitigate steel corrosion in acidic solutions, employing corrosion inhibitors is a practical approach. [1-2-3]

In this study, we investigated the corrosion inhibition properties of a novel organic phosphonic acid (DTMP) on carbon steel exposed to 1 N H_2SO_4 at 30 °C. The molecular structure of DTMP played a crucial role in its selection, as it features multiple phosphonic functional groups and heteroatoms (nitrogen).

The inhibitory effectiveness of DTMP was assessed using potentiodynamic polarization curves and electrochemical impedance spectroscopy (EIS). Furthermore, we evaluated the kinetic and adsorption parameters associated with the corrosion inhibition process.

The presence of DTMP on the metallic surface was confirmed through scanning electron microscopy (SEM), while the elemental composition of the carbon steel was analyzed using energy dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). Additionally, the impact of temperature on the corrosion rate was explored. Both kinetic and standard thermodynamic parameters were computed and thoroughly discussed.

Experimental results demonstrated the effectiveness of compound as a corrosion inhibitor for steel in 1N H_2SO_4 solution, with inhibition efficiency increasing proportionally to inhibitor concentration. AC impedance measurements, analyzed using appropriate equivalent circuit models, provided insight into the corrosion inhibition mechanism. Surface analysis confirmed the formation of a protective inhibitor film on the carbon steel surface.

Keywords: Carbon steel; Organic phosphonic acid; Corrosion inhibition; Adsorption; Sulfuric acid

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C.O. 34

Preparation of hydrogels based on cellulose derivatives and study of the swelling rate of the films obtained

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Cellulose is the major component of biomass and one of nature's most abundant biopolymers, biodegradable and non-toxic [1, 2]. Carboxymethyl cellulose (**CMC**) which is derived from cellulose is an anionic, water-soluble, a linear polysaccharide of anhydro-glucose, with many applications in the food industry, in cosmetics, pharmaceuticals, detergents, etc. [3], due to its hydrophilic character and bio compatible property. Furthermore, the carboxylate groups of **CMC** are evolved in various chemical processes such as in situ gelation, bio adhesion, sensitivity to environmental stimuli and controlled drug release. Beside the **CMC**, the polyvinyl alcohol (**PVA**) is a polymer that can be also used to synthesize hydrogels, because it has hydrophilic, biodegradable and non-toxic properties.[4]

In this work, we are interested in the preparation and characterization of mixed hydrogels based on **CMC**, and **PVA**, with compositions ranging from 25/75 to 75/25 (w/w), using boric acid as a crosslinking agent. We are also concerned to study the swelling rate of the various films vs the hydrogel composition, in water, and in salty systems.

Keywords: hydrogel, carboxymethyl cellulose, reticulation, water retention

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C.O. 35

Green Williamson Enhancement of the Hydrophobic Properties of Cellulose Fibers: Thermodynamic Study and Application to Elaborate Rosemary Essential Oil (REO) Biodegradable Plastic Coacervates

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In this paper, the dispersion encapsulation was investigated as new process to elaborate the principal active (PA) loaded biodegradable plastic coacervates, which designs a model of vector system and drug delivery matrix. The Rosemary Essential Oil (REO) (~54 %w) was wrapped, as PA-model, in Benzyl cellulose acrylate (BCac, DS_{Bnz}~1.4 and $_{DSAcr}$~0.4) coacervates that elaborated in the dispersing aqueous phase as new cellulose derivative. The advantage of this modification is to ensure the transition from hydrophilic to hydrophobic character of the cellulosic shell during the encapsulation process, which leads to encapsulation in one step. Indeed, during the reaction, the dispersive forces, generated by the grafting reaction, disturb the hydrophilic character of the water-soluble cellulose acrylate (Cac0.4). Then, the hydrophobic behavior, acquired by the grafted benzylic entities, increases the BCac- affinity to the organic compounds (oily dispersed phase). Therefore, the migration of the resulting polymer chains to the EO-rich (discontinuous) micellar dispersed phase, to form a biphasic micellar membrane, is strongly suggested. Experimental investigations, such as the relationship between the degree of substitution (DS) and the demixing behavior of the polymer solutions, are in good agreement with the theoretical interpretations basing on *the Flory-Huggins thermodynamic theory*. The results showed a high DS effect on the physicochemical properties, especially the *molar Gibbs free energy* of mixing.

Keywords: Cellulose acrylate, Williamson, Encapsulation, Biodegradable plastic, Flory-Huggins, Thermodynamics of polymers.

C.O. 36

Influence of heating rate on combustion and kinetic analysis of biomass derived biochars produced via pyrolysis

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The objective of this study is to investigate of the heating rate and the type of the fuel, on the kinetics and the combustion behavior of peanut shell PS, sugar cane bagasse SC, and their solid biofuels respectively PS400 and SC400. The biofuels were produced by the pyrolysis process at a temperature of 400 °C/min for 2 hours. The combustion characteristics, such as the combustion process, the combustion index, and the ignition index were evaluated by the thermo-gravimetric analysis. Also, the kinetic parameters of all the samples were determined by using the Coats-Redfern method. The results have shown that the biomass raw presents higher reactivity and higher combustibility index, compared to the solid biofuels. Moreover, we've found that this characteristic increased when increasing the heating speed. On the other hand, for the kinetic parameters we notice that the activation energies decrease with the increase in the heating rate for the biofuels. Concerning the first stage of the biomass raw the activation energies decrease with the increase in the heating rate but for second area of the biomass of the two samples, we've found that the activation energies has increased with the increase in the heating rate.

Keywords: Pyrolysis; fuels; combustion; kinetic; heating rate

C.O. 37

Ecofriendly synthesis of cellulose-silver nanocomposite and the evaluation of their antibacterial activity

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Researchers are actively working on the development of innovative materials sourced from renewable and environmentally sustainable resources to generate valuable products. Over the past few decades, materials based on polysaccharides have emerged as highly promising options due to their abundant availability and ecological viability. Furthermore, their utilization across diverse fields has witnessed [1,2].

In this work, we report on a facile and environment-friendly microwave method to prepare cellulose/Ag nanocomposites using palm date wood extract as an effective reductant for silver ion onto surface of cellulose. In order to obtain cellulose microfiber (MFC) from date palm wood fibers, a succession of specific chemical treatments including alkalization and whitening treatment have been developed.

Cellulose obtained have been characterized by different techniques. FTIR spectra confirmed the removal of non-cellulosic components after chemical treatments and XRD confirmed the presence of cellulose pics.

Experimental results indicated that the palm date wood extract was an effective reductant for silver ions favoring the formation of silver with higher crystallinity and mass content in the nanocomposites.

Silver nanoparticles were identified within the cellulose matrix through Scanning Electron Microscopic (SEM). The FTIR characterization studies demonstrated the existence of silver in the cellulose nanocomposites. Additionally, the XRD analysis confirmed the formation of silver peaks within these composites.

Qualitative antibacterial tests towards gram negative (Escherichia coli) and gram positive (Micrococcus luteus) bacteria are carried out and the results demonstrated that the Ag-MFCs inhibit the bacteria growth, with 9–13 mm of inhibition zone for the both bacteria.

These results demonstrated that the Ag-MFC possess suitable and promising antibacterial behavior and could be used for industrial and technological application.

Keywords : Silver nanoparticles; cellulose-silver nanocomposite; Antimicrobial activity

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C.O. 38

Elaboration of the film based on recycled PET and EPS functionalized with phosphate nanoparticles using electrospinning

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The aim of this study is to develop a flame-retardant film based on recycled PET obtained from waste plastic water bottles and EPS collected from electronic packaging and functionalized by phosphate nanoparticles using the electrospining technique.

Different percentages of the phosphate nanoparticles (1%, 3%, and 6%) were added to improve the flame retardant properties of the developed films.

The surface chemistry of electrospun PET and EPS films was examined using Fourier transform infrared (FTIR) spectroscopy. The surface morphology of the pristine and functionalized films was investigated using scanning electron microscopy (SEM). The fiber diameter decreased considerably after the incorporation of the phosphate nanoparticles.

The vertical burning test was used to investigate the flame resistance of the functionalized film. It was observed that the treated film exhibited flame-retardant properties and did not burn completely after 5 s of flame application compared to the pristine films. The obtained residue increased with the addition of the phosphate nanoparticles. The thermal stability of the films based on PET and EPS was assessed by TGA, which showed thermal stability up to 100°C.

This research advances sustainable solutions through the use of recycled PET and EPS using the electrospinning technique.

Keywords: Electrospinning, recycled PET and EPS, Flame-retardant

C.O. 39

Ion-Matter Interactions in Nanostructured Organic Materials

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Ion beams are widely used in several scientific and technological domains. Particle bombardment spans a range of applications, such as introducing dopants into semiconductors, cleaning and smoothing surfaces, conducting reactive ion etching, etc.

The analytical techniques of Secondary Ion Mass Spectrometry and Secondary Neutral Mass Spectrometry (SIMS/SNMS) are particularly intriguing when applied to 3D chemical imaging of organic samples. Numerous conditions must be met in these techniques to enable the chemical analysis of organic materials. For instance, the primary kinetic energy imparted to the sample should, on the one hand, be enough to trigger molecular desorption and ionization, but on the other hand, it needs to be sufficiently low to prevent significant collision-induced damage.

The main difficulty lies in identifying conditions that meet all these requirements. A variety of primary ions, including monoatomic and cluster projectiles, have been explored. These projectiles employ diverse pathways for energy deposition and ejection processes when they impact. An intriguing avenue for advancing SIMS/SNMS methods involves using novel substrates, such as graphene.

The processes involved in molecular emission in poly(3-hexylthiophene) (P3HT) on silicon (100) and in phenylalanine molecules ($C_9H_{11}NO_2$) deposited on a free-standing bilayer graphene will be discussed. This discussion will be grounded on the results of the Molecular Dynamics computer simulations, obtained using low-energy He, Ar, and Xe projectiles, as well as argon gas cluster projectiles, respectively.

Keywords: sputtering, graphene, molecular dynamics, organic materials, mass spectrometry, monoatomic and cluster projectiles

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C.O. 40

Biodegradable block copolymers obtained by controlled polymerisation applied for wastewater treatment.

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This work was aiming at associating both expertises and thus combining to synthesize poly(ε-Caprolactone-block-poly(oligo(ethylene glycol)methyl ether methacrylate (OEGMA)) copolymers using a bifunctional initiator. Thanks to their POGEMA block, such copolymers may exhibit a lower critical solution temperature (LCST) in aqueous medium and self-assemble in aqueous aggregates with various morphologies, such as micelles or vesicles. This propriety is very promising for biomedical applications such as drug delivery or respect environment.

The two-step route for the synthesis of these copolymers is using either ATRP or ROP as first step and the other polymerisation secondly. Each polymerisation was studied carefully in order to control the macromolecular parameters of the copolymers. The ATRP of methacrylates bearing oligo(ethylene glycol) with different side-chains lengths was studied. Three different methacrylates were selected (MEO2MA, MEO5MA, MEO9MA). Their ATRP was carried out in solution in toluene at 70 °C from two different intiators (Ethyl 2-bromoisobutyrate as model initiator or 2-hydroxyethyl-2-bromoisobutyrate as bifunctional initiator). Copper(I) bromide and *N*-propyl-pyridylmethanimine were used as catalytic system with or without initial addition of copper(II) bromide. ε-CL was polymerized in solution using tin octoate, tin of tetrakis(phenylethynyl) and bismuth triflate as non-toxic catalysts.

Keywords: Biodegradable, thermo-sensitive, Ring-opening polymerization, Atom transfer radical polymerisation,

C.O. 41

Removal of the Colloidal Suspension from Dam Water Using Mineral Coagulants Prepared by Co-Precipitation

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In this work, we were interested in eliminating the organic and mineral compounds that pose problems in obtaining drinking water using the method of coagulation. These substances are stable in the medium due to their colloidal sizes and surface loads, which require appropriate treatment. For this purpose, we explored the removal of colloidal suspension using a coagulant formed by co-precipitation of $AlCl_3.6H_2O$ in an alkaline medium. This practice leads to the formation of polymeric species mixtures such as $Al_{45}O_{45}(OH)_{45}Cl$ and $Al_2O_3.H_2O$ after washing. The removal efficiency of mineral and organic matter is evaluated by measuring the turbidity and permanganate index by varying the concentration of the coagulant from 0.04 to 0.4 $g.1^{-1}$. It has been shown that the effectiveness of the treatment had been increased in parallel with the concentration. The preliminary hydrolysis of aluminium leads to a fixation of the pH throughout the concentration range. This character had solved the problem of direct use of aluminium salts (conventional method) resulting in a modification of the pH and subsequently, variable efficiency. The refined coagulant (after washing) reaches the removal of 97% turbidity and almost all oxidizable matter using only a mass of 0.08 $g.\ 1^{-1}$.

However, using the crude coagulant (without washing) containing a significant amount of NaCl requires 0.4 $g.1^{-1}$ to reach only 87% removal of turbidity as well as 35% of oxidisable matter, with an increase of conductivity compared with that of the refined coagulant.

Keywords : Coagulation . Polymer-aluminium . Colloidal suspension . Turbidity . Oxidisable matter

C.O. 42

Optimization of a Pyrolysis Reactor for Plastic Waste Conversion into Pyrolytic Oil: Analysis, Characterization, and Process Parameter Impact

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This study focuses on optimizing a pyrolysis reactor to convert plastic waste into high-energy-value pyrolytic oil. To achieve this optimization, finite element analysis (FEA) was conducted using the ANSYS software to design the reactor efficiently. Subsequently, the impact of temperatures and heating rates on the yields of the pyrolysis process was examined. Temperatures were varied between 300°C and 500°C, while heating rates ranged from 5 to 30°C/min. Liquid, solid, and gas fractions were observed as response parameters. Our results showed that moderate temperatures and slower heating rates favored the formation of the liquid fraction, with a maximum yield of 72% achieved in a temperature range between 365°C and 370°C at a heating rate of 10°C/min.

In summary, Fourier-transform infrared spectroscopy (FT-IR) and gas chromatography-mass spectrometry (GC-MS) analyses were utilized to characterize the plastic pyrolysis fuel, aiming to better understand its properties and composition.

Keywords: Pyrolysis, Reactor, Plastic waste, Finite Element Analysis

C. O. 43

Knoevenagel Condensation Catalyzed by Oil Shale-Based Support under Microwave Irradiation: A Sustainable Approach

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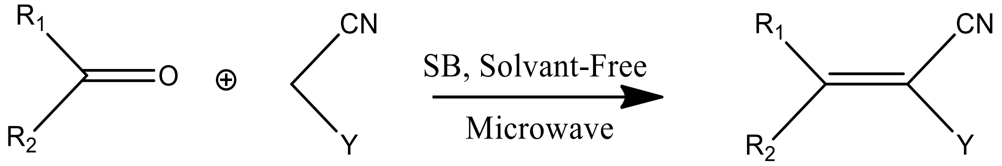
Knoevenagel condensation is a widely utilized organic synthesis method for the formation of carbon-carbon double bonds. However, traditional approaches often rely on toxic and costly catalysts. In this study, we explore the use of oil shale-based support as a catalyst for Knoevenagel condensation under microwave irradiation. The unique properties of oil shale, such as its porous structure and abundant surface functional groups, make it an attractive candidate for catalytic support. Microwave irradiation enhances the catalytic performance by promoting reaction kinetics. This sustainable approach offers several advantages, including reduced reaction times, improved selectivity, and lower energy consumption. The combination of oil shale-based support and microwave irradiation provides a greener and economically viable solution for Knoevenagel condensation of aromatic aldehydes with methylene compound.



Keywords: Oil shale, Microwave, Knoevenagel condensation, Aromatic aldehydes Active methylene compounds

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C. O. 44

Production of Biodiesel by transesterification reaction of sunflower oil with ethanol using nanoparticles mesoporous sulfated zirconia

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The limited resources of fossil fuels and the need to develop renewable energy sources are stimulating the development of alternative and sustainable energy sources derived from renewable feedstocks. In recent years Biodiesel which is considered as an important clean energy resource is receiving much attention. Many works have focused on the transesterification reaction of several varieties of vegetable oil by short chain alcohols on solids acid. Sulfated zirconia (SZ) considered as a superacid catalyst, generally leads to good yields but the major problem is its strong deactivation related to the loss of sulfate species. In this work, by adjusting preparation and activation conditions, sulfated zirconia present high performance for the transesterification of sunflower oil with ethanol was obtained. The synthesis of zirconia calcined at 500°C was carried out by hydrolysis of zirconium n-propoxide. The preparation of sulfated zirconia was performed by adding of sulfuric acid solution to $Zr(OH)_4$. The mixture was filtered and dried at 120°C, and finally calcined at 500°C. The amount of sulfur is about 2.9 wt. % and remains unchanged even after calcination at 500°C. The catalytic activity of ZrO_2 and SZ catalysts towards the transesterification reaction of commercial sunflower oil by ethanol was measured in a hydrothermal reactor equipped with a teflon chamber. Previously the catalyst was activated under nitrogen flow at different temperatures in the range 200°C to 400°C. The products were subsequently characterized by measurement of the viscosity, density, acid value and by ATR-FTIR spectroscopy. Addition of sulfate species improved the specific surface area of the catalyst (Zirconia : 80 $m^2.g^{-1}$; SZ : 168 $m^2.g^{-1}$), and stabilized tetragonal phase of zirconia. By SEM, nano-structure of particles was identified, for both samples, but adding sulfates to zirconia decreases the particles size. Before catalyst activation of SZ, the IR spectra shows the characteristic bands of bidentate SO_4^{2-} ions coordinated to Zr^{4+}. However, after activation of SZ at 450 °C a band at 3640 cm^{-1} appears attributed to bidentate (type II) OH groups accompanied by the band at 1398 cm^{-1} characteristic of highly covalent sulfates on the surface. IR-study of 2,6-dimethylpyridine (DMP) adsorption identified both Lewis and Brønsted acid sites on SZ whereas no Brønsted acid sites were detected on ZrO_2. DMP adsorption points out that the bidentate OH groups of SZ are highly acidic. Pure zirconia is inactive for the transesterification reaction. By contrast, SZ catalyst presents activity for biodiesel production with yield that increases with SZ activation temperature. Indeed, the best yield for biodiesel with acid value, density and viscosity characteristics respecting the requirements of EN14214 and ASTM D6751 standards is 87.6 % and is obtained after SZ activation at 400°C. These results are related to the nature of the ionic or covalent sulfate species on the zirconia surface and consequently to the Lewis/Brønsted ratio as a function of the activation temperature. The very high activity of the SZ catalyst can be related to the good dispersion of the surface sulfate species with a covalent character.

C.O. 45

Experimental investigations into the ecofriendly production of calcium acetate using Tarfaya oil shale as a promising and attractive source

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Calcium acetate is a widely used and much sought-after commercial product in various industrial sectors. It is used as a conservative or stabilizer in the pharmaceutical and agri-food sector, for both foodstuffs and animal feed. However, the calcium acetate production process based on lime rock is relatively energy-intensive, relying mainly on the use of calcium oxide and calcium carbonate. Herein, the primary aim of this study is to investigate the utilization of oil shale as a substitute raw material for the production of calcium acetate. The world's oil shale resources are vast and offer significant potential. They are currently attracting considerable renewed interest from the scientific community and are gaining importance in the energy sector [1, 2]. Oil shale is a highly abundant natural rock composed of organic matter tightly bound to a mineral matrix of carbonates, quartz, and clay. This rock can be valorized by using it as a source of energy or hydrocarbons for the production of carbon fibers or unconventional gas. However, the quantity of mineral matter, which represents over 70% of the raw Tarfaya's rock weight, constitutes a significant barrier to the development of this industry. Eliminating carbonates and enriching the rock in organic matter can considerably improve the process of industrial exploitation of oil shale.

This is the framework for the present study aimed to develop a green process to produce purified calcium acetate from shale. The yield of calcium acetate produced from the pretreatment of Tarfaya oil shale with acetic acid under mild conditions was around 48%, and its purity was comparable to commercial calcium acetate, while generating an oil shale concentrate rich in organic matter that can be used in the energy sector.

Keywords: Calcium acetate, oil shale, pretreatment, green process.

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C.O. 46

Adsorption and UV-light photodegradation of crystal violet, methylene blue and procion red dyes with novel orthoborate $Sr_2Ni(BO_3)_2$ nanoparticles

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A novel distrontium nickel diborate, $Sr_2Ni(BO_3)_2$ nanoparticles with an average size of 38 nm have been successfully obtained by solid-state reaction at 850 °C. The XRD patterns refinement shows that the cell parameters are a= 10.109(6)Å, b=5.432(2) Å, c=6.094(1) Å, and β=116.700(4)°, with space group C2/m. Infrared spectroscopy shows the existence of BO3 groups in $Sr_2Ni(BO_3)_2$. The microstructure of the studied borate consists of the nanotube’s shapes. The gap energy was calculated from the absorption spectrum for the direct and indirect band-gap (E = 3.92 and E = 4.44 eV) which is typical of the wide-band-gap. The studied borate was evaluated as a new adsorbent and a good candidate for the crystal violet (CV), methylene blue (MB) and procion red (PR) dyes for degradation from an aqueous medium, The study of the influence of the mass of the $Sr_2Ni(BO_3)_2$ catalyst showed the degradation of the three dyes, with a percentage of elimination that exceeds 90%. The kinetics data with UV and without UV irradiations for CV, MB and PR were well fitted with second-order kinetics. The overall experimental results suggested that this new orthoborate with adsorption and photocatalytic activities has a great potential for the treatment of water contaminated by toxic substances.

Keywords: Borates, Photodegradation, Adsorption, Optical properties

C.O. 47

Improving dielectric properties and energy storage capacities of BNT ceramics through glass modification

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An innovative approach was adopted to improve the energy storage and dielectric properties of BNT ceramics by incorporating a glass additive. alkaline-phosphate-based glass was chosen for its optimal dielectric properties intended to enhance the overall energy storage performance of the dielectric ceramic. A specific chemical approach was adopted to minimize the alteration of the crystalline structure and the formation of impurities which is one of the main drawbacks of glass additive strategy. The XRD and Rietveld refinement results reveal the formation of a pure BNT phase with no secondary phases. The dielectric parameters were evaluated in the frequency range of 1 Hz to 1 MHz, over a wide temperature range of 30 °C to 270 °C, indicating miner variation in their values for the glass-ceramic composite with lower glass content. Simultaneously, our findings indicate a notable increase in the relative density with reduced grain size and the sintering temperature owing to the glass addition. Polarization (P-E) hysteresis loops demonstrate that the energy storage and energy efficiency of the BNT based glass-ceramics were enhanced in comparison to the pristine BNT ceramic. Their dielectric properties depend on the glass content. For instance, a glass-ceramic with an optimized glass content of 2.5 wt% shows the recovered energy of 154.9 mJ/cm^3 with an energy efficiency of 88.64%.

Keywords: Perovskite; Phosphate glasses; Glass-ceramic composite; Dielectric properties; Energy storage

C.O. 48

Understanding of electrical properties of phosphorus oxide-based glasses containing transition metal

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The all-solid battery is an approach advancement in battery technology, representing a revolutionary improvement. All-solid batteries use solid inorganic chemicals to facilitate lithium-ion diffusion, unlike typical Li-ion batteries, which transport ions between electrodes via liquid electrolytes. This approach encourages research into new families of solid electrolytes with high ionic conductivity similar to liquid electrolytes, as well as strong mechanical and thermal durability. For this purpose, novel lithium phosphotungstate glasses and glass ceramics were prepared using the solid-state technique, with properties such as density, molar volume, free volume, and packing density thoroughly assessed. The structural approach is studied using infrared (IR) spectroscopy and the results show that the chemical substitution induces various structural unit changes. Electrical conductivity measurements of the glasses are investigated using the impedance spectroscopy technique over a wide frequency range and at varied temperatures. It is determined that the alkali concentration affects electric conductivity. At room temperature, the dc conductivity reaches 10^{-6} ($\Omega^{-1}.cm^{-1}$) with the activation energy of 0.20 eV. The frequency dependence of the glass conductivity is investigated, and the correlated barrier hopping (CBH) mechanism governs conduction.

Keywords: Phosphate; Glasses; Glass-ceramic; Structure; Conductivity

C.O. 49

Ordering Degree and Magnetic Transitions in $La_2Ni_xCo_{1-x}MnO_6$ Compounds

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The structural and magnetic properties of the new double perovskite oxides $La_2Ni_xCo_{1-x}MnO_6$ (x = 0.2, 0.25, 0.5, 0.75, 0.8) [1] are investigated using X-ray powder diffraction and squid magnetometry. The X-ray powder diffraction data shows that all the compounds crystallize in the monoclinic structure with space group $P2_1/n$ at room temperature, the cell parameters decrease gradually as substituting Ni^{2+} by Co^{2+}, due to the smaller ionic radius of Ni^{2+} (0.69 Å) compared to Co^{2+} (0.74 Å), the elementary structure indicates that the cations $(Co/Ni)^{2+}$ and Mn^{4+} are octahedrally coordinated with the oxygen atoms, the $(Co/Ni)O_6$ and MnO_6 octahedra are connected by O_1 and O_2 along a and b axis, and by O_3 along c-axis. The magnetic studies for all the compounds have been performed in both DC and AC magnetic fields in the temperature range from 2 to 300 K. All samples exhibit a main paramagnetic to ferromagnetic (PM-FM) transition between 232 K and 260 K, and their Curie temperature increases rapidly with increasing x values. Three samples with x=0.2, 0.25 and 0.5 respectively display also a secondary PM-FM transition between 200 K and 208 K. The ordering degree for the five double perovskites has been calculated, the results show that the Ni^{2+}rich double perovskites (x=0.75 and 0.80) have a high degree of ordering (>96%), while the oxide with x=0.25, the lowest degree of cation ordering. The thermal variation of out of phase component of AC susceptibility presents also frequency-dependent transitions between 65 K and 110 K unfolding the existence of super-paramagnetic mono-domains in all samples.

Keywords: Double perovskites, Spin glass transition, Disorder, Paramagnetic-ferromagnetic transition, Super-paramagnetic.

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C.O. 50

Unveiling the Multifaceted Nature of Sr_2XMoO_6 (X=Fe,Cr) Double Perovskites: Insights into Electronic and Optical Properties

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This study investigates the electronic and optical properties of double perovskite materials Sr_2FeMoO_6 and Sr_2CrMoO_6. We analyze charge transport mechanisms and electronic structure using electrical conductivity measurements. Dielectric function analysis reveals the materials' absorption characteristics and their relation to the electronic band structure. These findings provide a comprehensive understanding of these materials, paving the way for potential applications in optoelectronic and thermoelectric devices. This work contributes to the development of new functional materials in solid-state physics.

Keywords: Double perovsites, DFT, Electronic and Optical Properties, GGA approximation.

C. O. 51

Strontium substitution effects on the crystal structure, microstructure, optical and electronic properties of $Ba_{2-x}Sr_xBB'O_6$ (B/B'= Ti, Mn, Zr) double perovskites

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Various studies carried out since the fifties to the present, have revealed that the materials with perovskite structure exhibited a wide variety of physical and structural properties [1, 2]. But probably the reason that determined the intensification of studies on these compounds, is the discovery in recent years, for some of them the colossal magnetoresistance effect [3], studies for understanding and improving these properties are conducted all over the world. In this context, considerable interest has focused in recent years on double perovskites type $A_2BB'O_6$ (A= Ba, Sr, Ca… ; B = Ni, Mg, Fe, Zn … ; B'= W, Mo, Te… ; or B/B' = Ti, Mn, Zr).

In this work, we report that the compositions in the system $Ba_{2-x}Sr_xBB'O_6$ (B/B'= Ti, Mn, Zr) with $0 \leq x \leq 0.25$, were synthesized by the solid state reaction in polycrystalline form by thermal treatment, in air. Crystallographic analysis was performed by Rietveld refinement of experimental X-ray diffraction patterns. Results show that the solid solution system $Ba_{2-x}Sr_xBB'O_6$ (B/B'= Ti, Mn, Zr), remains as cubic perovskite in the marge of $0 \leq x \leq 0.25$, with $Pm\bar{3}m$ (no. 221) or $Fm\bar{3}m$ (no. 225) space group at room temperature. The surface characteristics and microstructure of the samples were studied by SEM images, while micrography and composition were determined by EDS analysis. Vibrational properties of the compounds were studied by FTIR spectroscopy. Furthermore, UV-visible spectroscopy technique was employed to study the optical properties and band gap of the obtained double perovskites.

Keywords: Double perovskite, Synthesis, Crystal structure, Rietveld refinement, Optical properties, Electronic properties.

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C.O. 52

Sensor based on a 1D photonic crystal for the detection of hydrochloric acid in water for water quality monitoring

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When it comes to avoiding water's harmful impacts on human health, hydrochloric acid (HCl) detection is essential. Necessary actions include preserving drinking water quality, safeguarding the environment, keeping an eye on industrial activities, and conducting routine monitoring and early identification of their occurrence.

The objective of this study is to determine the presence of hydrochloric acid in water by exploiting the sufficiently sensitive transmission of various visible and near-infrared wavelengths through our one-dimensional photonic crystal. The transmission characteristics of the proposed design were examined using the Transfer Matrix Method (TMM) in MATLAB.

The suggested model can be utilized not only for detection but also for figuring out how much hydrochloric acid is present in the samples under investigation. This is because, depending on the concentration of hydrochloric acid, our model transmits a single wavelength that reflects this concentration. The remarkable sensitivity of our detector is demonstrated by the variation of the transmission peak (transmitted wavelength) from a simple change in concentration.

Keywords: 1D photonic crystal, sensor, hydrochloric acid, sensitivity, transmission properties, TMM.

C.O. 53

5V spinel structure materials as positive electrode of Lithium-Ion Batteries for electric vehicles (EV)

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Nowadays, the extend use of the wireless electronic devices, in addition to the need to solve the problem of the global warming by the generation of sustainable energies and the use of electric vehicles (EVs), led to an increase demand for energy storage technologies. Batteries are widely used since the past decade as they represent the best technology to answer this increasing demand.

Among all types of batteries, lithium-ion ones (LIBs) are dominating the market of the electronic devices and the electric vehicles. Such systems require a continuous improvement and development of their components to achieve safer and more efficient accumulators. One of their most important components is the positive electrode. Many cathode materials have been developed since the introduction of layered $LiCoO_2$ by Sony in 1992, including the olivine $LiFePO_4$ and the spinel $LiMn_2O_4$.

During REMCES-13, we will present the synthesis of spinel structure materials with general formula $LiMn_{1.5}Ni_{0.5-y}M_yO_4$ (M = Cr, Fe and Co) with different compositions of the M metal transition (MT). The aim of this work is to prepare M-based LNMO spinels with excellent electrochemical performances, especially, at high rate capability. This latter feature is considered as an important property to develop rechargeable batteries with high power densities suitable for applications such as electric vehicles (EV) and hybrid electric vehicles (HEV). To achieve this aim, the study of the influence of the MT content on the electrochemical performances and the effect of the particle size will be presented and special attention will be given to the study of the behavior of the prepared materials at high rate capability.

C.O. 54

Valorisation de l'acide phosphorique industriel dans l’élaboration d'électrodes pour batteries haute performance et économiques

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Le Maroc, engagé dans une politique énergétique visant à accroître la part des énergies renouvelables à 50 % de sa production électrique d'ici 2030, met l'accent sur la nécessité de développer des solutions efficaces de stockage d'énergie. De plus, le développement très rapide de l’électronique portable (micro-ordinateurs, téléphones mobiles, caméscopes, etc.…) et des véhicules électriques, ont suscité une très forte demande en générateurs électrochimiques rechargeables (batteries au lithium et sodium) à haute densité d’énergie, permettant une autonomie suffisante pour une masse et un encombrement réduits. Dans ce domaine, la tendance actuelle vise à améliorer les systèmes précédemment cités, en recherchant des électrolytes stables et plus surs, mais surtout des matériaux actifs de point de vue électrochimique, facile à mettre en œuvre, conduisant à des générateurs de puissance massique et d’énergie spécifique élevées.

L’élaboration de nouveaux matériaux d'électrode pour ces batteries représente une opportunité majeure, notamment en tirant parti des ressources minières nationales telles que les phosphates. L'utilisation de l'acide phosphorique technique, issu de l'industrie des phosphates, dans l'élaboration de matériaux phosphatés pour le stockage d'énergie, ouvre de nouvelles perspectives pour la valorisation de ce sous-produit industriel, contribuant ainsi à l'effort national pour une transition énergétique durable.

Dans cette optique, notre étude est concentrée sur l'élaboration d'un matériau phosphaté, en particulier le phosphate de lithium et de titane $LiTi_2(PO_4)_3$, qui présente un potentiel intéressant comme anode dans les batteries Li-ion. Nous avons examiné l'utilisation de trois types d'acide phosphorique : un acide purifié servant de point de référence, l'acide phosphorique industriel produit par le groupe OCP dans sa forme brute, et une version de cet acide que nous avons soumise à un prétraitement en utilisant un matériau naturel à la fois économique et écologique.

Quelle que soit l'acide phosphorique utilisé, le matériau phosphaté obtenu a été caractérisé par plusieurs techniques d’analyse : DRX, ATD-ATG, ICP et MEB. Enfin une étude électrochimique a été menée sur les trois électrodes négatives obtenues par les différentes sortes d’acide phosphorique, afin de mettre en évidence d’éventuelles modifications structurales au cours de cyclage.

Mots-clés : Acide phosphorique, Prétraitement, Matériaux pour électrodes, Batteries Li-ion, Stockage d'énergie.

C.O. 55

Enhanced cycling performance of $LiNi_{0.5}Mn_{1.5}O_4$ cathode material with a truncated octahedral shape for Li-ion batteries through Ti doping

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High-voltage $LiNi_{0.5}Mn_{1.5}O_4$ is considered a prevalent cathode material for lithium-ion batteries owing to its abundant material resources, low cost, and eco-friendliness [1]-[2]. Different approaches were proposed to improve the electrochemical performance of LNMO-based batteries, including morphology control, surface modification, and element doping [3]-[4]. In this work, we successfully prepared pure LNMO and Ti-doped LNMO spinel materials using a straightforward sol-gel method. The crystal structure, morphology, and electrochemical properties of the prepared samples were investigated using X-ray diffraction, Raman spectroscopy, and high-resolution scanning electron microscopy, as well as charge-discharge/cyclic voltammetry tests. From the X-ray diffraction profiles, it was found that all samples crystallized in a pure cubic spinel structure with a $Fd\bar{3}m$ space group. Moreover, LNMO and Ti-LNMO exhibited truncated octahedral shapes. For the electrochemical results, the doped sample exhibited high working potential and excellent cycling stability, with an initial specific charge/discharge capacity of 165/108 $mAh.g^{-1}$ at a rate of 0.1C, and an initial Coulombic efficiency of 65%. After 100 cycles, the specific charge/discharge capacities were found to be 104/102 $mAh.g^{-1}$ at a rate of 0.1C with a Coulombic efficiency of 98 %.

Keywords: LNMO; Ti-LNMO; Sol-gel method; cathode materials; high voltage; Lithium-ion batteries.

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C.O. 56

Biochar from rosemary waste: a renewable resource

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Morocco stands out as one of the world's leading producers of rosemary essential oil. The extraction of this oil results in substantial volumes of solid waste, presenting an opportunity for recycling into valuable materials. Consequently, this study aims to assess the effect of biomass origin (rosemary stems or leaves) and pyrolysis temperature (400-900°C) on biochar characteristics. It highlights structural diversity, paving the way for diverse applications including biodiesel production, soil amendment, and wastewater decontamination. XRD, IR, SEM, complex impedance, DSC and CNHSO are used for the chemical and physical characterization of all samples.

The results revealed that stem biochars are different from leaf biochars, and biochars obtained at $T<700°C$ are different from those obtained at $T≥700°C$. The XRD analysis of biochars revealed two broad peaks situated at 24° (2θ) and at 44° (2θ). These peaks correspond to the (002) graphite basal plane and the (100) plane perpendicular to the basal plane graphitic structure reflection, respectively [1]. Quartz (SiO_2) has been systematically found in all biochars, which can give them added value in biodiesel production, catalytic industries and retention for wastewater decontamination [2]. SEM revealed that the surfaces of the biochars displayed crater-like structures of uniform diameter, originating from the release of volatile molecules during the emptying of glandular trichomes and epidermal cells [3]. As the pyrolysis temperature increased, both types of biochars exhibited a decrease in O/C and H/C ratios, signifying a reduction in polarity and an increase in hydrophobicity [4]. The O/C and H/C ratios of stem biochars are lower than those of leaves. For $T≥700°C$, the conductivity σ decreases sharply with frequency, involving a translational motion with a sudden hopping [5].

Keywords: Rosemary waste, Pyrolysis, Biochar, Biodiesel.

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C.O. 57

Cellulose from agricultural waste: production and application

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In recent years, there has been a notable increase in the exploration of new renewable and non-conventional sources to produce biodegradable nanomaterials. Nature harbours valuable cellulose-rich materials that have so far been under-exploited and can be used to create cellulosic derivatives like cellulose microfibres (CMFs) and cellulose nanocrystals (CNCs).

In this study, the main objective was to extract cellulose nanocrystals (CNCs) from agricultural waste using methods that are both efficient and sustainable. To achieve this high-quality extraction, we followed a well-defined protocol involving several key steps.

The extracted cellulose nanocrystals were subjected to in-depth characterization using advanced techniques such as thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (DRX).

The resulting nanocrystals have crystallite size 7,5 nm and have high thermal stability, and high mechanical strength, which makes them suitable for a variety of applications, specifically as reinforcements for composite materials.

Key words: agricultural waste, cellulose nanocrystals, nanomaterials, composites materials.

C. O. 58

Adsorption of lead ions from aqueous solution by moroccan oil shales

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In light of the escalating soil contamination and the pervasive presence of toxic heavy metals in domestic, agricultural, and industrial emissions, there is an urgent demand for cost-effective and eco-friendly natural absorbents to mitigate impurities.

The oil shale in the Rif region of northern Morocco, while previously valued primarily as an energy source, has now garnered significant attention for its potential as an alternative material in environmental applications, especially in the treatment of certain liquid effluents. These shale deposits exhibit varying chemical compositions across different locations, encompassing both inorganic and organic constituents.

In this study, we explore the utilization of raw oil shale deposits from the Rif region as bio-sorbents to mitigate lead toxicity in the environment. Our findings indicate that Pb2+ was adsorbed at a rate of 20 mg/g from wastewater, with the efficiency of the elimination process closely tied to physico-chemical parameters such as pH, contact time, initial concentration of the adsorbate, and mass of the adsorbent. Furthermore, we investigated the interaction between lead ions and crude oil shale using kinetic models and adsorption isotherms, revealing that the employed oil shale-based bio-sorbents exhibit effectiveness in environmental decontamination efforts.

Keywords

Lead ions, raw oil shales, biosorbants, wastewater, environmental.

C.O. 59

Synthesis of a low-cost adsorbent from Ziziphus jujube stones for removing dye from wastewater

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Ziziphus jujube, a Mediterranean species renowned for its culinary and medicinal applications, also yields substantial waste by products that necessitate valorization. In response to this opportunity, agricultural waste from Ziziphus jujube stones emerges as a cost-effective and readily available solution for dye adsorption due to its affordability and effectiveness. The objective of this study is the synthesis and utilization of a low-cost adsorbent derived from Ziziphus jujube stones for the removal of methylene blue (MB) from wastewater. Initial analyses employing Fourier transform infrared spectroscopy (FTIR), X-ray diffraction, Scanning Electron Microscope (SEM), and Energy Dispersive X-ray Spectroscopy (EDX) offer a comprehensive characterization of MJS. Furthermore, the investigation systematically explores the impact of adsorbent dosage, contact time, temperature, initial concentration, and pH to optimize adsorption capacity. Experimental findings reveal that the MJS adsorbent effectively removes approximately 94% of the MB under batch mode and room temperature conditions. This dual-purpose approach not only addresses the challenge of agricultural waste management but also offers a sustainable solution for wastewater treatment.

Keywords: dye, adsorption, jujube, wastewater treatment.

C.O. 60

Perspectives of our research activities on chemical synthesis and modeling

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In the course of our academic research activities we carried out different chemical synthesis and modeling in the aim to discover various appropriate uses with perspectives of creating useful technology for the society. The methods that we have used to achieve such a fundamental work range from the spectroscopy- and chromatography experimental techniques to the theoretical chemistry ones. In this presentation we will review how our practical and theoritical chemical analysis have contributed to the local (Beni Mellal-Khénifra region) research and development in various domains of : i) agriculture products (quality protection of virgin olive oil), ii) medical care in collaboration with local hospital (urinary crystals and urinay stones, and prevention of urolithiasis), iii) for sustainable development we investigated the recovery of dyes like methylene bleu and methyl red using our local organic products as we succeeded to extract these dyes by adsorption on lignocellulosic materials [1]. Materials derived from niobochromates, presenting the structure of tetragonal tungsten bronzes, are endowed with dielectric properties which would serve technological applications such as those of the minaturization of electronic devices and hightech applications [2]. Thus, the study of the solid state of synthesized and real matrices has allowed us to valorize natural resources, bio-concretions and very important materials for different applications for the benefit of the well-being and the so-called general security of populations around the world.

Keywords: Solid state, bio-concretions, depollution, photovoltaics, valorization, dilectric, well-being.

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C.O. 61

Flame Retardancy and Water Repellence Enhancement on Cotton Fabric via Titania-Boron Sol-Gel Technique

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The objective of this work was to prepare various sols using Titanium (IV) butoxide (TBT) and incorporating boric acid as a functional additive. These sols were then applied to cotton textile fabric using the pad-pry-cure method. Fourier-transform infrared (FTIR) spectroscopy and scanning electron microscopy (SEM) were used to analyse the resulting cotton textiles and evaluate their chemical composition and surface morphology. The study demonstrates that TiO_2-boron-based coating was successfully applied to the surface of the cotton fabric. X- ray diffraction analysis showed that the fabric's crystallographic structure was not affected by the coating. The treated cotton samples were evaluated for thermo-oxidative stability, burning behaviour, drop absorption, and water uptake. The study found that using a TiO2-boron-based sol-gel coating with a 2.5 molar ratio of boric acid resulted in excellent heat stability and flame retardancy. The cotton fabric treated with TiO2-boron-based coatings demonstrated self-extinguishing properties. Additionally, the fabric's water-repellent properties were enhanced, resulting in improved drop time and reduced water absorption compared to untreated fabric. The effect of these coatings on the mechanical characteristics of cotton samples, as well as their washing fastness were studied. Furthermore, the functionalized cotton fabric can be used in many fields and industrial applications for aesthetic and protective reasons.

Keywords: Coating, surface modification, textile cotton fabric, Sol–gel, Boric acid, tania sol, Flame retardant, water repellent

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C.O. 62

Synthesis, characterization, and utilization of a lignin-based adsorbent for effective removal of methylene blue and methyl orange dyes from aqueous solution

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In order to identify more efficient and environmentally friendly adsorbent materials, the present study extensively investigated the adsorption phenomenon of Methylene Blue (MB) and Methyl Orange (MO) on magnetic lignin beads. For this purpose, lignin was isolated from Solanum Elaeagnifolium Cavanilles Weeds and treated using a solid-state approach. Then, the prepared beads samples were characterized by SEM, EDX, XRD, FTIR, TGA, and zeta potential measurement. The adsorption of the mixture ions, the effect of time, pH, and initial pollutants concentration were methodically examined in batch experiments. According to the results, the highest adsorption capacity obtained shows a very interesting, which was considerable compared to other modified magnetics beads capacities cited in the literature. Furthermore, the removal mechanism of MB and MO was examined based on the characterization results before adsorption and also based on the kinetic results. It was concluded that cation exchange and electrostatic attraction between magnetics beads and the mixture ion mainly contributed to the adsorption process. These findings highlighted that magnetics beads offer many prospects for the removal of divalent metals from aquatic solutions.

Keywords: Lignin, Decontamination, Beads, Methylene blue, Methyl orange.

C. O. 63

Immobilization of heavy metal ions, Cd^{2+}, Hg^{2+} and Pb^{2+} using calcium phosphate materials

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Heavy metals are the main inorganic pollutants in wastewater produced by industrial activities related to mining, oil refineries, petrochemical plants and metallurgical industries. Given their toxicity and persistence, if these pollutants are inadvertently released into nature, they can cause serious damage to flora and fauna. As they are not biodegradable, their heavy metal content will tend to increase through bioaccumulation and can suddenly reach devastating thresholds. When it is not possible to completely remove heavy metals from such wastewater, it becomes necessary to implement a process that converts these inorganic pollutants from their labile forms into insoluble phases, making them unavailable for further accumulation. This article demonstrates the effectiveness of using calcium phosphate materials to immobilize heavy metal ions by ensuring their conversion from solutions into insoluble phases identified as heavy metal phosphates. It shows that when tricalcium phosphate or dicalcium dihydrate are exposed to separate solutions of Hg^{2+}, Cd^{2+}or Pb^{2}, a transfer of the heavy metals contained in the solutions occurs towards the solid phosphates. Analysis of solutions and solids produced after different times of exposure of phosphates to heavy metal solutions, performed by inductively coupled plasma mass spectrometry, X-ray diffraction and infrared spectroscopy, indicates that the transfer of metal ions to solid phosphates involves two mechanisms. A mechanism occurring during the first stages of exposure corresponds to a simple exchange between the metal ions of the solutions and the calcium ions of the solid phosphates leading to the incorporation of these metal ions into the phosphates. The second mechanism occurs when exposures are prolonged and involves the dissolution of the initial phosphates and the precipitation of new metal phosphates.

Keywords: Calcium phosphate; Heavy metals, Ions exchange; Dissolution-Precipitation

C.O. 64

From a material of construction to a material of pollutants removal, Clinker@HTS as an adsorbent of orthophosphates in the aqueous medium: Analysis of the adsorption phenomenon and Process Capability study

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One of the environmental problems presented is the excess of phosphates in ecosystems and their accumulation. Phosphate-rich discharges into aquatic environments mainly produce the phenomenon of eutrophication. As a result, this reduces the biodiversity of ecosystems and causes its degradation such as the disappearance of fish due to the oxygen depletion of the water.

The objective of this work is to propose, using an experimental and statistical approach, an effective adsorption process based on a composite having an adsorbent power of orthophsphates.

In order to study the adsorption phenomenon of orthophsphates in solution, a composite between Clinker and Hematite–titaniferous sand (Clinker/HTS) was developed.

The effect of the physicochemical parameters on the adsorption process such as the pH of the solution, the mass of the adsorbent, the contact time, the initial concentration and the temperature is highlighted. Modeling of adsorption kinetics shows that the pseudo second order model is best suited to describe the adsorption kinetics. Practically after 30 min of contact pollutant/support, we can eliminate 90% of PO_4^{3-}.

The study of the adsorption isotherms as well as the thermodynamic study have shown that the phenomenon of adsorption of orthophsphates on the composite can be correctly described by the Langmuir model. The adsorption results show that the adsorption capacity for the prepared composite reaches 34,43 mg-PO_4^{3-}/g.

The study of the capability of the adsorption process of orthophosphates on Clinker/HTS has shown the studied process is capable and satisfactory confirmed by the values of the following indices C_p=1,2 and C_{pk}=1,06.

Keywords: Environment, Process capability study, eutrophication, orthophsphates, adsorption, Hematite–titaniferous sand.

C.O. 65

From Waste to Resource: Developing Low-Cost Porous Carbon Adsorbent from Anaerobic Digestate for Dye Removal

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This study explores the dual benefits of treating food waste through an integrated approach combining anaerobic digestion and adsorption, aimed at ecological sustainability and economic efficiency. Utilizing food waste, the anaerobic digestion process under mesophilic conditions (38 °C) produces a significant amount of methane, showcasing a pathway towards renewable energy. The resultant digestate was utilized as raw material to design a low-cost porous carbon adsorbent. This novel adsorbent is evaluated for its efficacy in removing methylene blue (MB) from aqueous solutions, demonstrating an impressive adsorption capacity of 303 mg. g^{-1}. The adsorption process was found to fit best to the Langmuir isotherm and pseudo-second-order kinetic models, indicating effective dye removal through monolayer coverage and chemisorption. This study not only highlights the potential of food waste as a resource for energy and pollution mitigation but also contributes to the advancement of circular economy principles by offering a sustainable solution for water purification.

Keywords: food waste, anaerobic digestion, digestate, porous carbon, adsorption, dye removal.

C.O. 66

Free-standing surfactant-free plasmonic nanostructures at water/hydrophobic interfaces

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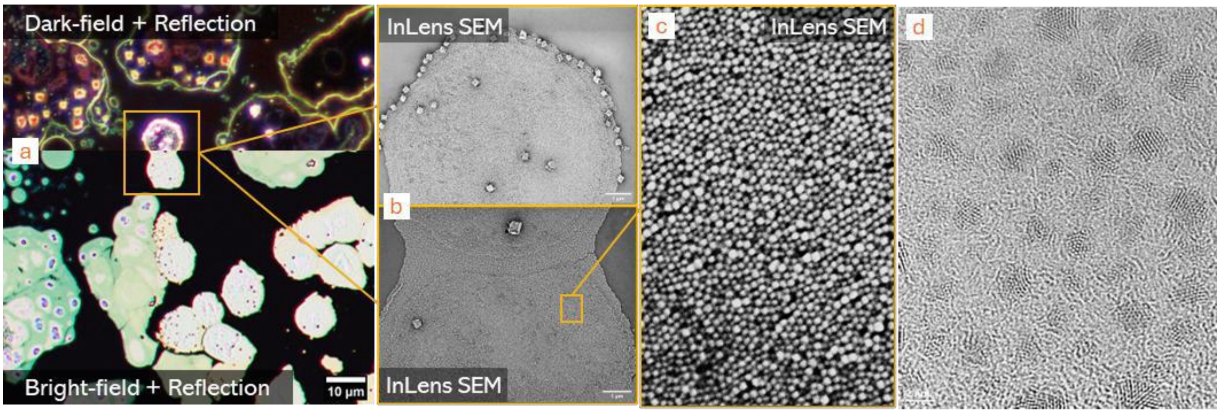
Although chemical synthesis of nanoparticle assemblies allows control of shape, size, and interparticle distance, their plasmonic response is greatly altered by the presence of surfactants and other impurities at the nanoparticle surface. Complete removal of the surfactant and other precursors is therefore essential but difficult to achieve, especially for high-sensitivity detection in Raman spectroscopy.



Interface silver film: (a) Optical microscopy and (b) SEM reveal cellular structures. Monodispersed 15-nm AgNPs in a domain (c). TEM shows even smaller AgNPs (~2 nm) (d).

To address this high-purity requirement, we developed a new synthesis leading to free-standing, surfactant-free silver nanostructures. Optical microscopy revealed that the film contained domains of varying color that correlated with the size of the nanoparticles observed by SEM. These domains can reach as wide as hundreds of microns of monodispersed 15-nm AgNPs. EDS and XRD confirm that the films consist of silver. Organization of the AgNPs into either hexagonal configurations or lines can pertain to the beginnings of large-scale organizations such as the cellular, floral, cubic, and fractal nanostructures observed on the films.

TEM of the free-standing film revealed even smaller NPs (~2.5 nm) under the beam without coalescing. UV-Vis and DLS also confirm the stable presence of AgNPs in the aqueous media of the system despite the absence of surfactants.

Keywords: AgNPs, nanostructures, water/hydrophobic interface

C. O. 67

Forced process deactivation of industrial catalysts used in the SO_2 to SO_3 oxidation reaction in the sulfuric acid production unit.

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An experimental procedure for the forced deactivation of representative sulfuric acid catalysts has been developed to gain a good understanding of the deactivation mechanism of industrial catalysts in a shorter time span, i.e. a maximum of 4 hours. Indeed, the efficiency of the commercial V_2O_5-M_2SO_4/SiO_2 catalyst used for H_2SO_4 production can progressively decrease over time. Around 8 years of service can lead to inactivation. Catalyst deactivation is generally assimilated to chemical, mechanical and thermal mechanisms. The experiments in this study were carried out using an experimental test bench to study forced deactivation by steam. This study takes into account various parameters such as the initial flow rate of N_2 gas, which acts as a water vapor carrier, and the flow rate of SO_2 gas. These flows must be precisely controlled by millimetric valves, with SO_2/N_2 ratios equal to 0.84 and 1.65. The water bath temperature is maintained at 80°C, the reaction temperature. Finally, the total reaction time is also taken into consideration. This parameter plays a very important role in the deactivation of industrial catalysts. At the end of the study, the deactivated catalyst was characterized by X-ray diffraction (XRD) and compared with the new catalyst to observe a structural change between the two catalysts, marked by the disappearance of several peaks. This result is confirmed by catalytic tests to investigate the reactivity of deactivated catalysts using iodometric assay in the context of SO_2 oxidation to SO_3. The aim is to compare the percentage of SO_2 converted between the new catalyst, which represents 63%, and the deactivated catalyst with an SO_2/N_2 ratio of 1.65, showing a significant drop down to 37%. This research aims to deepen our understanding of the catalyst deactivation mechanism, which could have a significant impact on the sulfuric acid production industry.

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C.O. 68

Carbon nanotubes as nanoreactor for catalytic applications

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The aim of this work is to evaluate the performance of hydroxyapatite as a catalyst support for the synthesis of carbon nanostructures. We also investigated the possibility of using the carbon nanostructures [1] thus produced for two distinct applications: as a catalyst support [2] and as a support for the growth of octocalcium phosphate, $Ca_8H_2(PO_4)_6,5H_2O$, a material with a composition close to the mineral composition of bone. For application in catalysis, we have studied the selective hydrogenation of aromatic compounds on ruthenium-based catalysts deposited on carbon nanotubes or nanofibers [3-5]. Finally, with regard to the growth of octocalcium phosphate on hydroxyapatite-carbon nanostructures composites. The composite materials produced could find application in the biomedical field. The present work lies at the intersection of catalysis and nanotechnology.

Keywords: CVD, carbon nanostructures, hydroxyapatite, catalysis, ruthenium, composites.

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C.O. 69

Theoretical study of facial selectivity induced by atropoisomerism and regioselectivity in the [3 + 2] cycloaddition reaction of benzonitrile oxide with 5-methylenehydantoin by the DFT method

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The [3 + 2] cycloaddition (32CA) reaction between benzonitrile oxide (BNO) and 5-methylenehydantoin (MH) was investigated using the MEDT perspective at the DFT/B3LYP/6–31 + g(d,p) level of theory. The topological analysis of the ELF reveals a zwitterionic character in this 32CA reaction, and the non-polar nature is evident from the global electron density transfer (GEDT) calculations at the transition states (TSs), consistent with calculated high relative free energies. The predicted regioselectivity and atropisomerism induced facial selectivity towards the anti-isomer aligns perfectly with the experimental results. In the 32CA reaction, the activation energy is linked to the generation of non-bonding electron density at N2 nitrogen and a pseudoradical center at C3. Notably, the formation of new C–C and C–O covalent bonds was not observed at the TSs, in agreement with the calculated total electron density and the positive Laplacian of electron density at the bond critical points observed at the interatomic bonding regions of the TSs.

Keywords: MEDT, Benzonitrile oxide, Methylenehydantoin, ELF, NCI

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C. O. 70

The optoelectronic characteristics of Ru-complex sensitizers dyes for applications using dye-sensitized solar cells (DSSCs): A Quantum Chemical Approach

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Dye-sensitized solar cells (DSSCs) have emerged as promising alternatives to conventional silicon-based photovoltaic devices due to their cost-effectiveness and potential for efficient light harvesting. Ruthenium (Ru)-complex sensitizers are crucial in enhancing the light absorption and charge transfer processes within DSSCs. Understanding the optoelectronic properties of these sensitizers is essential for optimizing device performance. In this study, we employ time-dependent density functional theory (TD-DFT) to investigate the electronic structure and optical properties of Ru-complex sensitizers used in DSSCs. Through comprehensive computational analysis, we elucidate these sensitizers' molecular orbital configurations, absorption spectra, and excited-state properties. Our main objective is to identify key parameters that determine the potential applicability of these modified structures in photovoltaic cells. These parameters include properties like open-circuit voltage, energy gap (bandgap), and maximum absorption wavelength. Insights gained from TD-DFT calculations provide valuable guidance for the rational design and development of novel Ru-complex sensitizers with enhanced photovoltaic performance. This research contributes to the advancement of DSSC technology by offering deeper insights into the fundamental mechanisms governing light absorption and charge generation processes in these photovoltaic devices.

Keywords: DFT, TD-DFT, solar cells, gap energy, absorption wavelength.

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C. O. 71

Exploring the Structural and Electronic Characteristics of Rutile SnO2: A Multi-functional DFT Study

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The structural and electronic properties of rutile-type SnO2 were investigated using plane-wave pseudo-potential density functional theory (DFT) with various exchange-correlation functionals as implemented in the Quantum Espresso code. Twenty-five functionals were considered in the calculations, employing ultrasoft pseudopotentials. Our computational results demonstrate that the structural properties calculated with the PZ and VWN-RPA exchange-correlation functionals are very close and more consistent with available experimental data compared to other methods. However, the band gaps obtained from each functional are generally smaller than the experimental value of 3.6 eV [1]. Nonetheless, the numerical values obtained using DFT+U show promising results. Additionally, to understand the optical properties of the rutile phase of SnO2, we calculated the complex dielectric function and other optical properties considering Norm-conserving (NC) pseudopotentials.

Keywords: SnO2, DFT, DFT+U, Exchange-correlation functional, electronic structure

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C. O. 72

Molecular modeling of quercetin adsorption on kaolinite surface

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The design of drug delivery systems requires a safe and effective approach to combat serious diseases such as cancer and COVID-19 [1]. Major challenges in this field include cytotoxicity, bioavaibility, functionality, incorporation and drug release. Quercetin is known for its anti-inflammatory and antioxidant properties, making it an attractive candidate for the treatment of various diseases [2].

This study aims to use the adsorbent properties of (001) and (00-1) kaolinite surfaces to improve the targeted delivery of quercetin. Kaolinite is a stable, low-cost, non-toxic and environmentally friendly clay [3]. Molecular modeling was used (software Materials Studio 2020) to assess the adsorption performance of quercetin on the (001) and (00-1) kaolinite surfaces. Adsorption energies were calculated using density functional theory (DFT). The results indicated that the position of quercetin exerts a more significant influence on the adsorption interaction than the adsorption position on the kaolinite surfaces. By carrying out an analysis of the Mulliken population, the difference in electron density and the electron density of the states on the optimal adsorption system, the nature of the binding and the types of interaction were able to be determined. Indeed, the finding revealed that interaction of quercetin on kaolinite surfaces was controlled by both hydrogen bonding and electrostatic attraction.

Key words: Kaolinite, Adsorption, Molecular modulization, Quercetin, Interaction.

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C.O. 73

Computational Analysis of Plant-Derived Alkaloids : Exploring Their Potential Against Malaria Through Molecular Docking, Molecular Dynamic and ADMET Assessment

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Malaria remains one of the most devastating diseases, affecting millions of people worldwide each year. Plasmodium falciparum, the deadliest malaria parasite, is responsible for the majority of malaria-related mortality. The use of alkaloids against malaria focuses on harnessing natural chemical compounds found in certain plants to combat the disease. Alkaloids, such as quinine extracted from the cinchona bark, have historically been used to treat malaria. These substances disrupt the life cycle of the parasite responsible for the disease. Over time, other alkaloids have been discovered and studied for their effectiveness in malaria treatment, including synthetic drugs based on natural active principles [1]. The use of these alkaloids in antimalarial treatments is crucial for reducing the prevalence of the disease and saving lives in malaria-affected regions. However, drug resistance is a growing challenge, and research continues to explore new avenues to combat this deadly disease. In this study, we selected several alkaloids from various plant families to investigate their pharmacological activities, followed by an ADMET study to analyze how these compounds interact with the body. We also studied the biological activity of these compounds on certain essential malaria proteins by molecular docking. Next, a molecular dynamics study was carried out for the compound with the highest protein affinity energy, to investigate their stability. We utilized several software programs, including Gaussian 09, AutoDock Vina, Chimera UCSF, Pymol and Discovery Studio, to to carry out our work. All compounds were optimized using the DFT-B3LYP method. The results obtained in this study indicate that some of the compounds studied in this work may be potential drugs to combat malaria.

Key words: Malaria, Alkaloids, Docking, ADMET, Molecular Dynamic, DFT.

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C.O. 74

Green Energetic Material: Ammonium Dinitramide (ADN) for Space Propulsion and its Decomposition Mechanism.

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In recent years, there has been considerable interest in advancing the development of a new generation of high-performance solid rocket propellants. Among these, the ammonium salt of dinitramide acid $NH_4N(NO_2)_2$ (ADN) has garnered widespread attention as a potentially valuable energetic oxidizer for rocket propellants.

Its appeal stems from the production of clean and environmentally friendly exhaust products. ADN decomposes in the temperature range of 130 to 230 °C, accompanied by an overall heat release of 240 (±40) kJ mol-1.

This study explores the theoretical decomposition of ADN through Density Functional Theory (DFT) calculations using Gaussian 09 software and visualized by the GAUSSVIEW program. The investigation into the decomposition mechanism of ADN and the identification of the Transition State (TS) are detailed.

In this work, we also conducted a study regarding ADN decomposition to calculate energies, Mechanism, and Transition State (TS) using the standard 6–31G (d, p) basis set and the B3LYP functional under different conditions (Spatial Condition) such as: temperature variation, solvent change...

The comprehensive findings contribute to the understanding of ADN's behavior, expanding the knowledge base for the formulation and optimization of advanced rocket propellants.

Keywords : Ammonium Dinitramide, Propellant decomposition, Mechanism

C.O. 75

Thermochemical calculations to monitor the fate of heavy metals during solid waste incineration

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Over the preceding decades, thermodynamic methodologies and computations have been extensively employed in scrutinizing diverse processes, as well as in monitoring and innovating emerging technologies. The progression of novel methodologies is imperative to meet the energy demands of humanity, optimize the utilization of raw material resources, execute measurements for pollution prevention, and ensure environmental protection. These endeavors inherently necessitate preliminary analyses grounded in established thermodynamic models. Consequently, thermochemical calculations have been instrumental in appraising diverse processes, as well as facilitating the genesis of novel materials and technologies.

The types of application of thermochemical calculations can be summarized as follows:

- Advancement of novel high-temperature technological methodologies;
- Systematic optimization of chemical processes, encompassing the synthesis of refractory materials and microelectronics constituents;
- Rigorous examination of material stability under elevated temperatures and diverse environmental conditions;
- In-depth investigation into the chemical intricacies inherent in power-generating facilities, including nuclear plants;
- Streamlining the utilization of raw materials and implementing effective waste management strategies;
- Comprehensive analysis of burning by-products and industrial gas emissions, addressing their impact on the atmosphere;
- Formulation and implementation of processes designed to prevent environmental contamination;
- Exploration of mineral genesis processes, the formation of planetary bodies, and atmospheric dynamics of stars and planets, as well as other geo- and astro-chemical phenomena.

Our investigation centers on the application of thermochemical calculations utilizing the HSC Chemistry Chemical Reaction and Equilibrium Software in the context of waste incineration and the assessment of the destiny of heavy metals. The waste under consideration encompasses metals such as Cu, Zn, and Pb. Thermochemical simulations were conducted under conditions of thermodynamic equilibrium. Our analysis delves into the impact of chlorine content, as well as the effects of temperature and pressure, on the fate of the aforementioned heavy metals.

Keywords: Thermochemical, calculations, HSC Chemistry, waste, incineration, heavy metals.

C.O. 76

The Influence of Core Size on Nanoindentation Behavior of Nanoparticles using Molecular Dynamics Simulation

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Bimetallic nanoparticles serve as high-performance materials across various fields, owing to their ability to be structured in diverse configurations. These configurations combine noble-metal nanoparticles, commonly employed as catalysts in numerous applications, with 3d-transition metals, which are increasingly recognized for their potential in noble-metal-based catalyst integration [1]. It's crucial to acknowledge that the efficacy of these nanoparticles is intricately tied to their mechanical attributes, encompassing elasticity, stiffness, rigidity, hardness, and strength. Understanding these properties necessitates advanced characterization techniques such as in situ microscopy, spectroscopy, and computational simulations, among others [2]. In this context, molecular dynamics simulations are utilized to investigate the mechanical response of nanoparticles with varying core sizes and a range of grain sizes within the nanocrystalline shell. The analysis reveals that the hardness of core-shell nanoparticles (CSNPs) is significantly influenced by the presence of grain boundaries within the shell structure, in conjunction with the specific composition of the core materials. Furthermore, it is observed that normal CSNPs exhibit higher Young's modulus values, indicative of greater stiffness, whereas the inclusion of nanocrystalline phases in the shell leads to more flexible mechanical behavior. This study underscores the potential for tailoring CSNPs compositions and grain sizes to engineer materials with desired mechanical properties, such as enhanced strength and toughness.

Keywords: Bimetallic nanoparticles, molecular dynamic, Palladium, nickel, cobalt, Compression, Nanoindentation, dislocations.

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C.O. 77

Grain Growth in Nanocrystalline Ni During Thermal Annealing: A Molecular Dynamics Study

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Nanocrystalline materials have attracted significant research interest within the field of materials science, particularly nanocrystalline nickel. Thermal annealing, a fundamental topic of research, plays a critical role in determining the evolution of grain size in nanocrystalline metals. In this study, we investigate the isothermal grain growth behaviors of nanocrystalline nickel, focusing on the effect of annealing temperature. Molecular dynamics simulations using the Modified Embedded Atom Method (MEAM) potential developed by Lee et al. **[3]** were employed to provide detailed atomic-level information on the microscopic mechanisms involved in grain growth. Previous studies have demonstrated that annealing temperature has a significant impact on the grain growth of nanocrystalline metals. For instance, Sim˜oes et al. **[4]** observed significant grain growth in nanocrystalline copper thin films with increasing annealing time and temperature. Chojnowski et al. **[2]** found that annealing nanocrystalline chromium at temperatures above 400°C led to controlled grain growth. Chen et al. **[1]** reported a decrease in the frequency of annealing twins in highly rolled pure nickel as annealing temperatures increased. In this study, atomistic simulations were conducted to investigate the grain growth mechanisms, grain boundary structure, and the effects of annealing temperature on microstructural properties during grain growth. The models were constructed using the Voronoi geometrical method to study the grain growth mechanism. Our findings reveal that during thermal annealing, nanocrystalline nickel exhibits stacking faults, twinning, changes in grain size, rotations, and translations, which facilitate crystalline growth and grain coalescence. Grain boundary migration, grain rotation mechanisms, and dislocations (or stacking faults) were identified as intermediate mechanisms in the grain growth process. These results provide insights into how annealing temperature controls the rate of grain growth and its impact on the appearance of different types of defects during the growth.

Keywords: Thermal annealing, Nanocrystalline metals, Grain growth, Grain Boundaries, Nickel, Molecular dynamics

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COMMUNICATIONS PAR AFFICHES

C. A. 1

Elaboration et caractérisation physico-chimiques des verres du système $PbO-Fe_2O_3-V_2O_5$

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Les verres de vanadium ont fait l’objet de nombreuses recherches scientifiques car ils présentent un intérêt majeur pour l’industrie du fait de leurs propriétés semi-conductrices. L'utilisation du vanadium dans le stockage de l'énergie solaire ou éolienne est primordiale.

Les verres contenant du fer ont également suscité un grand intérêt. Ils présentent une conductivité électrique élevée à température ambiante et il est connu que l'ajout de Fe_2O_3 dans les matériaux vitreux de V_2O_5 augmente la conductivité en raison de l'augmentation des atomes d'oxygènes non pontants.

Nous avons concentré nos objectifs sur le développement de nouveaux matériaux vitreux à base du vanadium et du fer en élaborant et en analysant le système ternaire $PbO-Fe_2O_3-V_2O_5$.

Le système vitreux de composition $xPbO-(1-x)Fe_2O_3-yV_2O_5$ a été préparé par une technique classique de trempe à l'état fondu. La nature amorphe des verres préparés a été confirmée par la technique de diffraction des rayons X.

L’étude de ce système peut offrir des propriétés thermiques, optiques, magnétiques, électriques et diélectriques intéressantes.

Mots-clefs : Verres Ferro vanadates, DRX, Spectroscopie IR, DSC, Propriétés magnétiques et diélectriques.

C. A. 2

Structural and Surface Changes of SiO_2 Flint Aggregates under Thermal Treatment for Potential Valorization

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In order to extend their use, controlled SiOH SiO_2 surfaces were fabricated and investigated. A study of the effect of heat treatment on the structural and surface changes of a natural flint SiO_2 aggregate subjected to chemical treatment was carried out. The obtained samples were subjected to thermal treatment at three different temperatures: 500, 700, and 1000 °C. The samples were investigated using different techniques. X-ray diffractions (XRD) were used to follow the structure's evolution with the heat treatment. The decrease in the FWHM of the SiO_2-(101) peak showed that the crystalline quality improved upon heating. This result was confirmed by Fourier transform infrared spectroscopy (FTIR). The morphology of the SiO_2 samples was characterized using a Variable.

Pressure scanning electron microscope (VP-SEM), revealing the presence of disordered needles of nanometric sizes (500 nm) on the surface of the grains, which could be eliminated by heating at higher temperatures. Furthermore, FTIR spectroscopy also confirmed that heating caused a reduction in OH groups on the surface. Thermogravimetry (TG) was used as the reference method to determine the hydroxyl group content. The OH groups found on the surface of the sample without and with heat treatment at 500, 700, and 1000 °C were 0.83, 0.44, 0.28, and 0.2mmol/g, respectively. This study allowed us to obtain a controlled SiO_2 surface and provides new insights into the use of SiO_2 flint surfaces for new applications as functional filler in polymers/asphalts composites.

Keywords: SiO_2 natural aggregate; valorization; thermal treatment; microstructure; surface silica; silanol SiOH; circular economy.

C.A. 3

Synthesis and physicochemical characterization of vanadate-based glasses

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The resemblance in the chemical formulas of P_2O_5 and V_2O_5 might lead one to believe that vanadate glasses would have properties similar to those of phosphates. However, the structure of vitreous V_2O_5 does not resemble that of vitreous P_2O_5 formed by PO_4 units, nor that of crystalline V_2O_5 which is formed by VO_4, VO_5, and VO_6 units. The glass structure is composed of VO_5 and VO_4 units interconnected by vertices.

This study presents the synthesis and characterization of Barium Vanadophosphate glasses using techniques such as XRD, FTIR, XPS... The amorphous state of the glasses was confirmed by X-ray diffraction. XPS and IR spectroscopy were used to study structural modifications in the glasses, revealing the formation of P-O-V and V-O-V bonds as well as VO_5 and VO_4 structural units.

Fitting of the $V2p_{3/2}$ spectra showed the presence of V^{4+} and V^{5+} oxidation states for all glasses, while deconvolution of the O1s peaks allowed us to track the evolution of oxygen bonding with other elements.

Keywords: Vanadate glasses, X-ray Photoelectron Spectroscopy, Infrared Spectroscopy

C. A. 4

Effect of Crystallization of Sodium Phosphate Glasses on the Enhancement of Electrical Properties

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In recent decades, storage technologies have received a lot of attention due to their prospective applications. The demand for efficient, sustainable, and cost-effective energy storage devices has sparked high interest in the development of next-generation batteries. All-solid-state sodium batteries (ASSSBs) are gaining popularity as a viable alternative to lithium-ion batteries for large-scale energy storage, thanks to their abundance, low cost, and environmental friendliness. However, the development of efficient and stable solid electrolytes remains a critical challenge, with many limitations hindering the practical application, especially the low ionic conductivity. In this study, we investigate the effect of glass crystallization on the enhancement of electrical properties and the feasibility of sodium phosphate-based glass-ceramics as good ionic conductors. The glassy samples were elaborated via a melt-quenching method, then crystallized at the temperature of crystallization (T_x), determined using Differential Scanning Calorimetry (DSC), to obtain the glass-ceramics. The glass-ceramics were characterized through various structural, microstructural and electrical analyses including X-ray diffraction (XRD), infrared (IR), Raman, scanning electron microscopy (SEM) and electrochemical impedance spectroscopy (EIS). The results garnered show that the glass-ceramic exhibits high sodium ionic conductivity compared to the pristine glass, along with good thermal stability.

Keywords: Sodium phosphate glasses ; Glass-ceramics ; Crystallization ; Ionic conductivity.

C. A. 5

Elaboration, structural characterization and UV–Visible spectra of phosphate glasses in the system CaO-Na_2O-PbO-P_2O_5.

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Phosphate glasses in the system CaO-Na_2O-PbO-P_2O_5 were prepared by conventional melt quenching technique and characterized by XRD, FTIR, density, molar volume (Vm), DTA, chemical durability and UV-visible spectroscopy. The introduction of the PbO oxide instead of Na_2O in the glasses strengthens the vitreous network, as shown by the increase of the glass transition temperature and the increase of the density [1]. This behavior is a result of the replacement of Na-O bonds by more covalent Pb-O bonds. The larger polarisability of lead oxide is responsible of the improved chemical durability of these glasses [2]. From the UV–Visible absorption studies, the values of the optical band gap, Eg, and Urbach energy, ΔE, were evaluated.

Keywords: phosphate glasses, DRX, density, molar volume, DTA, IR spectroscopy, optical properties and chemical durability.

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C.A. 6

Synthesis, structural characterization, Properties and chemical durability of phosphate glasses containing nickel

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Phosphate glasses belonging to the Na_2O-ZnO-NiO-P_2O_5 system are synthesized and characterized by different techniques. The amorphous state of the glasses was confirmed using X-ray diffraction analysis (XRD). The introduction of NiO instead of ZnO in the studied phosphate glasses strengthens the vitreous network, as shown by the increase of the glass transition temperature and the decrease of the molar volume and the improvement of the chemical durability. This result is due to the replacement of Zn-O bonds by more covalent Ni-O bonds. Fourier transform infrared (FTIR) spectroscopy show the evolution of the phosphate [1, 2] skeleton when the NiO content increases. Optical properties such as gap energy were also studied.

Keywords: Phosphate glasses, density, DTA, IR spectroscopy, optical properties and chemical durability

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C.A. 7

Manganese addition impacts on the structural and physical properties of calcium borovanadate glasses

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The advancement of technology and engineering has continued to develop in close relation with the development of new elaboration methods and new functional materials. In the present work, we report on synthesis and characterization of the new glass compound belonging to the borovanadate system. The glass samples were elaborated by the melt quenching method.

The impact of the addition of manganese on the various properties of the glass samples prepared was examined using a number of different analysis methods.

X-ray diffraction was used to demonstrate the amorphous nature of the prepared glass samples. The variation of the different physical characteristics as a function of Mn_2O_3 content was studied in terms of structural changes in the glass matrix. In addition, to verify the group constitution of our samples, a structural study has been performed by means of infrared spectroscopy (FTIR) and Raman spectroscopy.

Keywords: Borovanadate glasses; Manganese; DRX; Spectroscopic studies; physical proprieties.

C.A. 8

The structural and surface changes of SiO_2 flint aggregate under thermal treatment

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In this work, the effect of the heat treatment on the structural and surface changes of a natural SiO_2 flint aggregate attacked with KOH solution was studied. The attacked silica was subjected to thermal treatment at three different temperatures, 500, 700 and 1000 °C. The obtained samples were followed by means of different techniques. X-ray diffraction (XRD) was used in order to follow the evolution of the structure with heat treatment and the decrease of the FWHM of the SiO_2-(101) peak shows that the crystalline quality is improved upon heating. This result was confirmed by Fourier transform infrared spectroscopy (FTIR).The morphology of SiO_2 samples were characterized using scanning electron microscope (SEM), reveal the presence of hydroxyl groups on the surface of attacked flint, which can be eliminated by heating at higher temperatures. Furthermore, FTIR spectroscopy also confirmed that the heating causes reduction of OH groups on the surface. Thermogravimetry (TG) was used as a reference method to determine the hydroxyl group content. The total hydroxyl group content was calculated from the difference in the weight losses from heating at two temperatures (200 and 900°C). The OH groups obtained on surface for the sample without and with heat treatment at 500, 700, and 1000°C were about 0.83, 044, 0.28 and 0.2mmol/g, respectively. This study contributes new insights into the use of flint for new applications.

Keywords: SiO_2 Flint, Thermal treatment, Microstructure, Surface silica, Hydroxyl groups, Silanol SiOH

C.A. 9

Investigating Medium Range Order in Mg-Al binary metallic glasses: molecular dynamics approach

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In this work, we used molecular dynamics (MD) simulations in order to investigate the Medium-Range Order (MRO) in Mg-Al binary metallic glasses (MGs). The embedded atom method (EAM) has been adopted to accurately model the interatomic interactions. Various techniques such as radial distribution function (RDF), coordination number (CN) analyses and Gaussian fitting have been mobilized to comprehensively study the impact of cooling rate, composition and mechanical solicitations, on the structural properties at the MRO level. Our results reveal that the 1-atom connection mode is consistently dominant across all cooling rates. Moreover, as the cooling rate increases in the $Mg_{25}Al_{75}$ binary MG, the abundance of the 4-atom and 2-atom connection modes increases, while the percentage of the 3-atom mode experiences a slight decrease. Furthermore, we investigate the influence of composition on the properties of Mg_xAl_{100-x} alloys, demonstrating that the RDF peaks and connection modes are highly sensitive to variations in the Al concentration. Additionally, we explore the relationship between mechanical properties and connection modes during tensile deformation. The 3-atom connection mode exhibits superior hardness and stability, while the 4-atom and 2-atom connection modes offer increased flexibility. These significant findings enhance our understanding of MGs' structural evolution, stability and deformation behavior. Ultimately, this knowledge facilitates the design and optimization of tailored MGs for advanced applications.

Keywords: Molecular dynamics, binary metallic glasses, EAM, Medium-Range Order

C.A. 10

Structural disorder and Medium-Range Order in Monoatomic Metallic Glass

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The investigation of structural defects in a simulated monoatomic metallic glass was undertaken using the recently introduced quasi-nearest atom (QNA) structural parameter via molecular dynamics simulations. A higher number of QNAs surrounding an atom generally signifies a higher concentration of defects in proximity to that atom. Structural analysis unveiled a spatially heterogeneous distribution of QNA quantities. Moreover, a significant correlation between QNA and cluster connections, particularly those involving four-atom and three-atom, was observed.

Keywords: metallic glass; quasi-nearest atom; molecular dynamics simulations.

C. A.11

Evaluation of the properties of polypropylene matrix composites reinforced with sisal and glass fibers thermocompression

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Composite materials are meticulously crafted to fulfill precise needs across a range of uses. They consist of a mixture of two or more substances, each with its own composition, creating unique physical and chemical properties at a larger scale. This blending results in novel or improved characteristics that surpass those found in the individual components. Mainly consisting of various polymers, composite materials are more widely used and favored over metal and ceramic composites due to their cost-efficiency, easy manufacturing processes, and versatility in numerous fields, particularly in advanced medical applications.

The objective of this study is to fabricate polypropylene matrix composites reinforced with varying ratios of sisal and glass short fibers, aiming to enhance the properties of the resulting sheets. The study assessed the mechanical, thermal, and morphological characteristics of various polypropylene formulations reinforced with sisal and glass staple fibers. Selection among the available sisal and glass short fibers (sSGFs) was based on their superior mechanical performance, notable chemical resilience, and effective dispersion within the polypropylene matrix, as confirmed by SEM morphological analysis. Furthermore, analysis of mechanical properties revealed that increasing the content of both glass and sisal fibers in the polymer matrix enhanced the tensile and flexural moduli of the developed polypropylene- based composites. Consequently, this research offers promising insights into producing high- quality polypropylene components reinforced with sisal and glass staple fibers, which could find applications in diverse thermoset or thermoplastic composite systems for high-value purposes.

Keywords: Thermocompression, polypropylene matrix, natural sisal fibers, glass fibers, composite materials.

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C.A. 12

Electrochemical Exploration of Vanadate Glasses for Corrosion Prevention

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In the first part, we investigated the electrochemical behavior of vanadium ions derived from the hydrolysis of vanadate glasses in HCl (1M) using cyclic voltammetry. The results showed that the shape of the voltammograms is hardly modified by increasing the scan rate, and that the intensity of the oxidation peak of ions (V4+ to V5+) for all recorded voltammograms at different scan rates varies linearly with the square root of the scan rate. Thus, the formed species chemically reacts, and a low reduction peak associated with the oxidation peak is observed.

In the second part, we tested the validity of these glasses as inhibitors of ordinary steel corrosion in HCl (1M). This study was conducted using polarization curve plots and electrochemical impedance spectroscopy. The results were confirmed by spectrophotometric analysis and surface analysis.

Keywords: Vanadate glasses; Transition metal; Cyclic voltammetry; Electrochemical impedance spectroscopy; Polarization curve; UV-Visible spectrophotometry; SEM.

C. A. 13

Optical and structural characterization of glasses belonging to Na_2O-NiO-P_2O_5 system

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Transition metal phosphates glasses are studied for their numerous applications as nonlinear optical materials, lasers and luminescent materials [1-3]. Many investigations of glasses belonging to Na_2O-MO-P_2O_5 (M = Mn, Cu, Co) systems were reported [4-6]. In the continuation of our work on transition metal phosphates glasses, the present study aims to investigate the effect of Ni^{2+} ions on structural and physico-chemical properties of two new series of phosphate glasses in Na_2O-NiO-P_2O_5 system. The glass samples have been prepared by the classical melt quenching method and characterized by differential thermal analysis (DTA), X-ray diffraction, Fourier-transform infrared (FTIR), Raman, UV visible and by density measurements. Introduction of Ni^{2+} ions in phosphate glasses increases the cross-link density in the glass network and the glass transition temperature (Tg), and improves the chemical durability due to the formation of P–O–Ni bonds. The optical band gap energy and the Urbach energy were determined from absorption spectra. The decrease in optical band gap shows the presence of more non-bridging oxygens due to the presence of Ni^{2+} ions instead of Na^+ ions. CIE L*a*b* and RGB parameter values are in good agreement with yellow-colored materials. Preliminary optical results of the studied glasses suggest their use as bandpass filters and as yellow ceramic pigments.

Keywords: Ni/Na-Phosphate glasses, Raman/FTIR, UV-visible, Chemical durability.

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C. A. 14

Effect of Zinc oxide on the structure-properties of (35-x) Li_2O–x ZnO–15PbO–$50P_2O_5$ glasse

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Quaternary lithium zinc lead phosphate glass system with composition of (35–y)Li_2O–yZnO–15PbO–$50P_2O_5$ (y=0; 5; 15; 25; and 35 mol%) was successfully prepared using a conventional melt-quenching method. Their composition dependence of physical and spectroscopic properties such as density, molar volume, glass transition temperature and FT-IR spectra have been discussed in association with the effect of substitution of zinc oxide (ZnO) for lithium oxide (Li_2O). Thus, ZnO is assumed to play an intermediate role in a way that Zn^{2+} cation tends to break P–O–P bonds forming ZnO_4 units with covalent Zn–O bonds. The predominant structural units in all these glasses are metaphosphate $(P_2O_6)^{2-}$ groups. An incorporation model of ZnO into the glassy network is proposed.

Keywords: Phosphate glasses, Zinc oxide, DSC, density, Molar volume, Infrared spectroscopy.

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C. A. 15

Effect of SrO on the structure and properties of Na_2O–CaO–TiO_2–P_2O_5 glasses

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Phosphate-based glasses have shown their identity in the field of biomaterials compared with silica-based glasses, because of their dissolution rate[1], as well as a low melting point, a low glass transition and low softening temperatures [2]. To improve the bioactivity of phosphate-based glasses, it is more and more interesting to add elements such as Sr, Ca and Ti. These elements are that have biological effects in its ionic form, such as improving the solubility of biomaterials, anti-resorptive activity [3].

The goal of this work consists of the elaboration and characterization of new vitreous materials having bioactivity properties in the oxide system Na_2O–CaO-TiO_2—P_2O_5 and investigated the effect of Sr on the structure and properties of this phosphate glass system these glasses were prepared by the classical method of melting followed by quenching. The obtained glasses were characterized by XRD, DSC, SEM, EDS and FTIR and density measurements. The XRD results showed that all glass samples were fully amorphous, the obtained DSC analysis displayed an increasing of the thermal stability and an expansion of the vitreous network by introduction of strontium. Glass density diminished and molar volume raised up with increasing of Sr content, owing to a less densely packed glass structure. The reactivity of these glasses in the SBF solution (Simulated Body Fluid) was also reported.

Keywords: Biomaterials; phosphate glass; thermal stability; bioactivity; SBF; density.

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C.A. 16

Multifunctional doped bioactive glasses for bone tissue regeneration: characterization, bioactivity, and antioxidant assessment

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Bioactive glasses (BAG) have garnered significant attention over the last decades for their therapeutic effectiveness in bone tissue regeneration (BTR). They are considered as multifunctional biomaterial that not only induces apatite formation on their surface but also can exhibit additional biological functionalities through the local release of therapeutic ions in the defect site. Silica-based BAGs have long been the most studied category due to their high stability, diverse compositional range, and modes of synthesis. Nonetheless, new BAG compositions have emerged recently in the alternative systems that opened new research perspectives in the field of tissue engineering. By incorporating therapeutic ions, such as Zn, Cu, or Mg, these glasses can attain distinct biological properties of interest, such as antioxidant, antibacterial, antitumor, etc. In the present work, new compositions of doped BAG are presented for potential dual antioxidant and biomineralization properties. Comprehensive characterizations of these glasses through FT-IR, DSC, XRD, and SEM were conducted. In addition, bioactivity assessments and antioxidant activities were also performed. Results show that all doped glasses, at different percentages, exhibit an amorphous nature related to their disorganized atomic structure. FT-IR analysis indicates minor changes in the structural features of the glasses which can be related to the incorporation of the dopant in the glasses. In addition, all glasses were characterized by rapid biomineralization ability in Simulated Body Fluid (SBF) solution. This was confirmed by FTIR where new bands related to P-O vibrations were detected. Furthermore, the antioxidant assay indicated that doping glasses with XO_2 induced an H_2O_2 scavenging activity which was more pronounced with increasing doping content. In light of these results, XO_2-doped BAG can be considered as multifunctional biomaterials for bone tissue regeneration.

Keywords: Bioactive glass, doping, bioactivity, antioxidant, bone regeneration.

C. A. 17

Phosphate glass fibers and their application in the reinforcement of polyester matrix composites

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Phosphate glass fibers have recently garnered attention as potential substitutes for conventional glass fibers, signifying a significant shift in the field of composite reinforcement [1-2]. This study focused on the production and characterization of phosphate glass fibers (PGF) and examining their impact on reinforcing Polyester Matrix Composites. Phosphate glasses were elaborated and converted into fibers. For this purpose, which were then employed as reinforcement for thermosetting composite materials. Polyester matrices reinforced with short phosphate glass fibers (sPGF) at weight fractions ranging from 5wt% to 20wt% were manufactured using the contact molding technique. The mechanical and morphological properties of various sPGF-reinforced polyester systems were evaluated.

The choice of the phosphate glass fibers (PGFs) was made because of their interesting mechanical performance, their high chemical stability in different aqueous media (acidic and basic) with a tensile strength of 2230 MPa, and their high level of dispersion in the polyester matrix without any ad sizing as proven by SEM morphological analysis. The mechanical analysis of the developed composites showed that the tensile strength and flexural strength was increased from 11 to 43.8 MPa and from 10.9 to 45 MPa, respectively when 20 wt % PGF was used. In addition, the analysis of morphological properties shows good interfacial adhesion between polyester resin and phosphate glass fiber.

Keywords: phosphate glass fibers (PGF); polyester matrix composites; chemical durability; mechanical properties; morphological properties.

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C. A. 18

Les propriétés vibrationnelles et la relation des verres métalliques

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Dans ce travail nous allons étudier les propriétés vibrationnelles de verres métallique CuZr, notre objectif est de rajeunir notre verre pour extraire ses propriétés vibrationnelles tel que la densité d'état vibrationnelle ensuite interpréter les résultats à partir de celles de l'expérience.

C. A. 19

Safeguarding Water Resources: Hybrid Material Synthesis for Pollution Control

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The objective of this study is to address the issue raised by the presence of pollutants in waters discharged by human activities. These waters contain a variety of pollutants such as organic matter, heavy metals, and pathogens, which can have adverse effects on public health and the environment. Crystal violet, a cationic dye widely used in various industries, poses a danger when discharged into wastewater. By contaminating aquatic ecosystems, it disrupts biological processes and reduces organism diversity. Moreover, its presence in drinking water sources can pose risks to human health. Thus, the discharge of cationic dyes into wastewater compromises both environmental and human health.

To address this issue, we proceeded with the synthesis of a hybrid material based on polymer as an adsorbent, with the polymer representing the organic part and an oxide as the inorganic charge, using adsorption technique. Our aim was to remove cationic dyes from contaminated aqueous solutions. After optimizing the parameters influencing the dye's adsorption power, we characterized the obtained hybrid material using various analysis methods such as X-ray diffraction (XRD), UV-visible spectroscopy, Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy with energy-dispersive X-ray microanalysis (SEM/EDX). Kinetic study showed that our hybrid material has a strong affinity for this dye.

Keywords: Water pollution, Crystal violet, Hybrid material, Adsorption, Dye removal

C.A. 20

Synthesis of Fluor/Hydroxyapatite - C-S-H materials from blast furnace slag as cost-effective adsorbent for efficient anionic (Methyl Orange) dye removal

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Wastewater stemming from dyestuff production stands as a primary contributor to water pollution. Various approaches have been employed to address the remediation of such contaminated water. Presently, a promising method involves utilizing adsorption, employing an economical, abundant, and environmentally friendly adsorbent, such as slag. This method holds potential for efficiently mitigating the impact of dyestuff production wastewater on water quality. The present research focuses black and white slag from SONASID-Jorf steel in Morocco for prepare hydroxyapatite (HAP)/C-S-H (calcium silicate hydrate) and fluorapatite (FA)/C-S-H mixtures using blast furnace slag for adsorption applications, using Methyl orange (MO) as a model compound. The mentioned phases were successfully synthesized using activated slag with NaOH alkali activator through a wet precipitation method with a molar ratio of Ca/P = 1.67. Characterization through X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, and scanning electron microscopy (SEM) revealed the formation of the hydroxyapatite (HAP)/C-S-H and fluorapatite (FA)/C-S-H phases synthesized by wet precipitation method. The adsorption potential of (HAP)/C-S-H and (FA)/C-S-H mixtures for to adsorb methyl orange (MO) from aqueous solutions has been investigated. The study encompassed various factors such as initial dye concentrations, contact time, pH, sorbent doses, and the temperature of the initial dye solution. Adsorption isotherms, including Langmuir, Freundlich models, were employed to describe the adsorption data. The findings underscore the substantial of (HAP) /C-S-H and (FA) / C-S-H mixtures as effective adsorbents for the efficient removal of MO from aqueous solutions. This potential is rooted in their cost-effectiveness, strong thermal stability, outstanding adsorption performance, and ease of separation. These characteristics collectively highlight the viability of these mixtures as valuable tools in addressing water contamination issues involving MO.

Keywords: slag, methyl orange, hydroxyapatite, fluorapatite, calcium silicate hydrate

C. A. 21

Enhancing Carbon Dioxide Capture onto Zeolitic Material through an Integrated Metakaolinization Process

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In addressing the imperative need for sustainable strategies to counter the escalating levels of CO_2 emissions, carbon capture and storage (CCS) via adsorption on porous materials has gained prominence as a forefront technology due to its capacity for achieving substantial CO_2 uptake. Among the diverse landscape of solid adsorbents explored for efficient CO_2 capture, encompassing activated carbon, porous silica, zeolites, and metal-organic frameworks. Zeolite 4A emerges as a pivotal contender, demonstrating notable promise in the realm of CO_2 capture. This is attributed to its exceptional attributes, characterized by high porosity, thermal stability, and exceptional selectivity for CO2. In this investigation, we delineate a novel approach for the synthesis of Zeolite 4A through a hydrothermal treatment methodology employing kaolin clay as the primary raw material. Our inquiry integrates advanced characterization methodologies, including X-ray Diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy, Scanning Electron Microscopy (SEM), X-ray Fluorescence (XRF) analysis, N_2 adsorption-desorption isotherms, Thermogravimetric Analysis (TGA), and Carbon Dioxide Adsorption experiments, aimed at comprehensively probing the properties of the resulting material and their potential applications. Surface area and pore volume assessments were conducted utilizing the Brunnauer–Emmet–Teller (BET) method from nitrogen adsorption isotherms, revealing that the synthesized zeolite 4A exhibited enhanced BET surface area and micropore volume compared to previously reported counterparts [1]. In addition, we thoroughly conducted an examination of the synthesized zeolite's CO_2 adsorption capacity across varying pressure gradients and temperature conditions ranging from -20°C to 40°C. Our findings reveal that the synthesized zeolite 4A exhibits remarkable CO_2 adsorption abilities, attaining a capacity of 3.125 mmol/g at a pressure of 13 bar. This value represents an improvement capacity for zeolite 4A to date, compared to previous reports which indicated a capacity of 2 mmol/g at 13 bar [1]. This study provides crucial insights into the synthesis, characterization, and performance evaluation of Zeolite 4A as a promising material for CO_2 capture applications.

Keywords: Zeolite 4A, Hydrothermal synthesis, Kaolin, Carbon dioxide, Adsorption isotherm.

References: [1] *doi: 10.3390/ma12091536*

C. A. 22

Development of a new akermanite formula using Moroccan geomaterials: Synthesis, characterization and bioactive behavior

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The current study focuses on the development and characterization of bioceramics rich in akermanite using locally abundant dolomite and perlite. Various batches were prepared for cost-effective ceramic production using uniaxial pressing method and firing at 1250 °C for 2 h. The results indicate the presence akermanite as the main crystalline phase through the addition of natural perlite, up to a maximum of 30% by weight, along with minor traces of diopside and periclase. The experimental findings suggest that the sample M2-B (25% of perlite by weight) demonstrates optimized properties (in terms of technological, mechanical and microstructural characteristics) compared to the other samples tested. The optimized ceramic underwent an in-vitro test using SBF to assess its bioactivity, which confirmed its quality through the formation of apatite, indicating a successful development of the bioceramic in terms of both microstructure and composition after soaking in the SBF solution.

Keywords: Akermanite, Bioceramics, Dolomite, Perlite, SBF, Apatite.

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C. A. 23

Technological and dielectric investigations on ceramics based on Lizardite geomaterial

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This work focuses on characterizing lizardite clay mineral and studying the technological and dielectric properties of ceramics made from this geomaterial through experimental measurements. This mineral has not previously been evaluated for their physical and dielectric properties. Lizardite clay was extracted from the Beni Boussera region in Morocco and analyzed to determine its chemical composition, mineral phases, and thermal properties. Purification isolated the key mineral components, predominantly silica (47.16 wt%) and magnesia (31.21 wt%), along with clay minerals lizardite and chlorite. Ceramic test specimens were fabricated by uniaxial pressing, followed by sintering at temperatures from 900-1200 °C. Increasing sintering temperature was found to decrease porosity and water absorption while increasing density, shrinkage, and mechanical strength. Optimized dielectric properties were achieved with 1100 °C sintering, resulting in a dielectric constant of 1.33, dielectric loss around 0.08, and conductivity of 4.86×10^{-8} S/cm at high frequencies. The 1100°C ceramic specimens showed 17% porosity, 2.02 g/cm^3 density, 9.86% water absorption, and 19.3 MPa mechanical strength. Overall, the natural lizardite clay was successfully employed to produce ceramics with favorable technological, mechanical and dielectric properties using a controlled manufacturing process, demonstrating the potential of this geomaterial for ceramic applications.

Keywords: Lizardite; Magnesian silicates; Ceramic materials; Sintering; Dielectric properties.

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C. A. 24

Photocatalytic Characteristics of Glass Ceramic

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Glass-ceramics, produced through controlled glass crystallization, have become indispensable in daily life due to their versatile applications. Recent research has reexamined these materials, emphasizing their potential in critical environmental areas such as water purification, hydrogen generation, and bacterial disinfection, owing to their photocatalytic properties. These glass-ceramics offer significant benefits including shape and size flexibility, high stability in physical, chemical, and thermal aspects, ease of fabrication, and consistent performance, thus presenting immediate solutions to pressing environmental concerns.

Phosphate glasses are extensively utilized, and adding TiO_2 enhances their potential in photocatalysis. TiO_2, known for its photocatalytic abilities, boosts the glass's reactivity to light, initiating chemical reactions that facilitate the breakdown of organic pollutants, thereby contributing to air and water purification. Analysis of thermal, structural, and morphological aspects demonstrates that increasing the TiO_2 concentration in phosphate glass enhances its photocatalytic activity, accelerating the degradation of organic pollutants under light exposure. These findings highlight the positive impact of TiO_2 content on the environmental performance of the glass, paving the way for sustainable and innovative solutions.

In conclusion, glass ceramics, particularly those incorporating TiO_2, significantly address environmental challenges due to their multifaceted properties. Further research is crucial to optimize TiO_2 proportions and understand its nuanced effects on photocatalysis, thereby fully harnessing the potential of these glass ceramics for environmental applications.

Keywords: Recrystallization, Glass ceramics, Photocatalysis, Phosphate glasses

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C. A. 25

Studying of the slag addition and sintering temperature for the technological and mechanical properties of dolomite-based porous ceramics

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This study delves into creating porous ceramics using Moroccan dolomite as the primary raw material. Additionally, the impact of adding slag on the mechanical and technological characteristics of the final product is explored. The characterization process of the initial materials was extensive, including analyses of chemical composition (XFR), mineralogy (XRD), and thermal profiling (DTA-TG).

Various ceramic structures were fabricated using uniaxial pressing and sintering techniques at different temperatures up to 1300°C. The study examined the effects of sintering temperatures ranging from 1100°C to 1300°C on morphology, phase composition, technological properties (such as porosity, water absorption, density, and shrinkage), resistance to flexural stress, and chemical resilience. The optimal sintering temperature was found to be 1200°C, resulting in a range of porosity from 50.28% to 41.4%, a density ranging from 1.7g/cm³ to 1.89g/cm³, a water absorption range of 28.07% to 24.8%, and a shrinkage range of 1.55% to 6.25%. These ranges varied based on the amount of added slag. The experimental findings emphasized the beneficial role of slag in enhancing the overall quality of ceramic products, particularly their mechanical properties.

Keywords: Dolomite; Sintering ; Slag ; Ceramics ; Technological properties

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C. A. 26

Mechanical properties of low-cost ceramic membrane made from mining waste

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This work aims to elaborate new low-cost ceramic membranes, in order to valorize different types of wastes such as red mud RM (mining waste). We also seek to apply the desired membranes in different fields especially in wastewater treatment.

Firstly we characterized RM to determine its mineralogical, chemical composition and its thermal behavior. Several essays were done so that we can optimize the right composition. The ceramic membranes were fabricated using a hydraulic press method, the prepared mixture contains 80wt% of red mud, 10wt% of lime dust and 10wt% of paper ash, molded into a flat disk shape and heated to the desired temperatures (900-1100˚C).

The starting materials and the obtained ceramic membranes were analyzed using several characterization techniques such as: XRD, XRF, thermogravimetric analyses and MEB.

Many tests are applied allowing the high chemical stability confirmation as well as the mechanical resistance and the physical properties of each fabricated ceramic membrane.

Keywords: Ceramic membrane, Valorization, Mining wastes, Water treatment, Red mud.

C. A. 27

Low-cost ceramic membrane from marble waste: Characterization and optimization using experimental design.

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In the field of wastewater treatment, ceramic membranes have emerged as a promising technology due to their high filtration efficiency and durability. Unlike traditional polymer membranes, ceramic membranes are made from inorganic materials such as alumina, silica or other ceramic materials. They can withstand extreme operating conditions, such as high temperatures.

To produce a membrane with high porosity and acceptable mechanical strength with the minimum of experimentation, we opted for optimized the preparation conditions by adjusting the sintering temperature, time and as well as the rate of marble waste addition.In this study, the Response Surface Methodology (RSM), based on the Doehl-type experimental design, was used.

Various analytical techniques, including X-ray diffraction (XRD), X-ray fluorescence (XRF), thermogravimetric analysis (TDA-TG), scanning electron microscopy (SEM), and Archimedes principal testing, were used to investigate the properties of these ceramic membranes.

Keywords: Clay, Marble waste, Ceramic membrane, Experimental design.

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C. A. 28

Potential use of new bentonitic clay materials from the Rif Oriental, Nador-Morocco: Application in ceramic tiles

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This article explores the bentonite deposit in Rif Oriental, Nador-Morocco, conducting analyses in mineralogical, physicochemical, morphological, geotechnical aspects, and ceramic performance. Mineralogically, montmorillonite, K-feldspars, and plagioclase are the primary associations, with lesser amounts of calcite, dolomite, and quartz. SiO_2 and Al_2O_3 are the predominant chemical components. The deposit's swelling index and Atterberg limits vary widely, according to geotechnical data, although all samples show noteworthy swelling and plasticity characteristics. Ten representative bentonite samples (Oz 1-Oz 10) undergo ceramic assessment, showing good quality post-dry pressing and sintering at 1000°C, with exceptions of Oz 4, Oz 5, and Oz 8. As a result, the same production method is used to manufacture two mixtures (Oz M and Oz M1). The resultant ceramics are evaluated in terms of their morphological structure, porosity, macroscopic appearance, bulk density, water absorption, shrinkage, and tensile strength.

Keywords: Bentonite; Traditional ceramics; Technological properties; Sintering.

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C. A. 29

Development of ceramics materials based on modified apatite prepared by Sintering a mixture of Calcium Apatite and layered double hydroxides

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In recent years, the development of calcium phosphate and clay materials attracted a lot of interest. These materials show excellent performance as multifunctional materials for their promising applications in the fields of energy storage, catalysis, environmental protection, drug delivery, and material science. In this study, new ceramics based on modified apatite were prepared by sintering a mixture of calcium apatite and Layered Double Hydroxides (LDH) with various percentages. The precursor powders were prepared by the wet precipitation method. Characterization techniques such as X-ray diffraction (XRD), Fourier Transform Spectrometer (FTIR), and Scanning Electron Microscope (SEM) were used to characterize prepared materials and to study the effect of clay phase on sintered apatite.

The results showed that during the sintering process, the incorporation of clay ions into the apatite structure resulted in the formation of modified hydroxyapatite as a principal phase. The decomposition of calcium apatite leads to the formation of biphasic ceramics comprising hydroxyapatite and substituted tricalcium phosphate.

The prepared materials based on modified apatite can improve the mechanical and surface properties of the calcium apatite ceramics.

Keywords: Calcium-Apatite, LDH-Clay, Sintering, Modified-Apatite, Ceramics.

C.A. 30

Mechanical properties of Portland cement blended with high fly ash fraction activated by alkali sulphates

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The production of traditional cement consumes massive mineral resources and intensive energy. Considering these problems, the use of industrial by-products is essential to reduce disposal costs, mitigate environmental risks and ensure sustainable development. One of the best ways to reduce the environmental impact of the cement and concrete industry is to use supplementary cementitious materials, such as fly ash (FA), in binder mixtures. The materials containing FA exhibit a wide range of properties compared to Ordinary Portland Cement. When high FA contents are used as a cement replacement, the compressive strength of mortars is reduced. Therefore, such admixtures necessitate activation. This study reports the results of an experimental investigation to find out the effect of chemical activation of Portland cement blended with 40% by weight of class F FA.

X-ray fluorescence and X-ray diffraction were used to characterize the prepared samples. The compressive strength of the prepared mortars was also evaluated.

Two chemical activators were used in this study Na_2SO_4 and K_2SO_4. The activation with Na_2SO_4 leads to an increase in the reactivity of the blended cement. Activation with Na_2SO_4 contributes to a significant increase in strength at both early and later ages.

Keywords: Cement; Fly ash; Alkali Activation; Mechanical Strength.

C.A. 31

Advantages of using high limestone and pozzolan content cements in the production of Roller-Compacted Concrete

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In Morocco, the use of limestone fillers and fillerized sand in the composition of Roller-Compacted Concrete (RCC) for dam construction has been a common practice for many years. However, the availability of these materials at current and future construction sites is becoming increasingly rare.

To address this challenge, we sought substitutes for limestone fillers and fillerized sand in the composition of RCC. We chose to use limestone-rich cements (CPJ) and/or pozzolanic cements (CPZ) as substitutes. We prepared four different mixtures, two containing CPJ with 35% limestone at varying dosages, and two others containing CPZ with 45% pozzolans also at different dosages. The mechanical (compressive and flexural strength) and physical (porosity and density) performances of these mixtures were compared to those of a reference formula containing limestone fillers and fillerized sand.

The results indicate that the use of both types of cements provides satisfactory compressive strengths at 28 and 90 days. Furthermore, extrapolation of the results to the long term suggests that reduced dosages of both cements are sufficient to achieve the minimum strengths of 10 MPa (minimum prescribed value for dams in Morocco) from the age of 3 years. Additionally, the densities of the four RCC formulas were found to be perfectly suited for the construction of large structures such as dams.

Keywords: RCC dam, fillers, limestone and pozzolanic-enriched cement, mechanical performance, physical performance.

C.A. 32

Influence of different chemical activators on the physical, mechanical, and microstructural properties of binder based on coal gangue and fly ash

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In recent decades, researchers have focused on replacing novel binders with traditional binders, such as lime and cement. The majority of researchers employ ecologically friendly binders that have a lower carbon footprint during the production process. On the other hand, the storage of waste from the mining industry, such as coal gangue and fly ash, poses a significant risk of environmental damage. Due to their high alumino-silicate concentration, they may be a promising alternative/substance as a precursor in alkali-activated materials (AAMs) production.

AAM is one type of binder that may provide an effective alternative to traditional binders. Alkaline activation of coal gangue and fly ash is of great interest in the context of new and environmentally friendly binders with similar properties or that improve the characteristics of conventional materials. Similarly, phosphoric acid-activated binders have the potential to be a superior mechanical performance and high temperature-resistant construction material.

This study presents a comparison between three chemical activators (NaOH, Na_2CO_3, and H_3PO_4) on the physical, mechanical, and microstructural properties of binder based on coal gangue and fly ash. Different molarities of NaOH, Na_2CO_3, and H_3PO_4 (5M, 8M, and 12M) are used to elaborate cubic samples (50 mm x 50 mm x 50 mm) based on activated coal gangue and fly ash. The samples are cured at 60 °C for 24 hours and then left at room temperature. Conforming to the standardized guidelines outlined in ASTM C 109/C 109M-08, compressive strength (Rc) is used to assess the mechanical properties of cubic samples at 3, 7, and 28 days of curing. Physical characteristics, such as bulk density, apparent porosity, and water absorption, are determined using Archimedes' principle, following specifications outlined in ASTM C 642-06. X-ray diffraction (XRD), infrared (IR), and thermogravimetric analysis (TG-DTA) are used to characterize coal gangue, fly ash, and samples based on coal gangue and fly ash.

Keywords: Coal gangue, Fly ash, Alkali-Activated Material, Alumino-silicate gel, Alkaline activation, Acid-activated binder.

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C.A. 33

Performance study of spent radioactive resins conditioning using cementitious binders incorporating red clay

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The Kingdom of Morocco has a 2 MW research reactor (TRIGA MARK II) and an interim storage facility at the Maamoura Nuclear Research Center (CENM), managed by the National Center for Nuclear Energy, Science, and Technology (CNESTEN), designed for radioactive waste management and treatment on a national scale. Spent radioactive resins (SRR) are commonly used to clean and treat water pool reactors in the nuclear industry. Cement binders are considered as the major matrices for the solidification/ of these kinds of radioactive wastes. Previous works from our laboratory have shown that blended cement incorporating red clays can potentially yield high-performance cement binders for encapsulation of SRR at a pilot scale (Z.Faiz et al.,2019). (wet base) within the cement binders were performed. The obtained results were compared to those of the waste forms carried out using the formulation with 8.3% of SRR adopted by CNESTEN and the formulation with 18% of SRR resulting from previous studies (A.Sadiq et al., 2022). The compressive strength and the porosity of SRR forms were improved after 28 days of curing time. These results suggest that the developed cementitious binders incorporating clay are a potential matrix for the solidification of these radioactive wastes.

Keywords: Cement binders, Spent radioactive resins, Solidification/encapsulation; clay additives;.

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C.A. 34

Development of Biphasic Biological Cement: Nanoapatite / Granules of porous βTCP

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Apatite self-setting cements are widely used as bone substitutes due to their biocompatibility and bioactivity. However, their low porosity and partial solubility limit their biodegradation and bone formation.

This study aimed to produce a novel apatite cement composed of high porous tricalcium phosphate (βTCP) granules dispersed within the apatite matrix. The cement was firstly prepared by the addition of an aqueous solution to a mixture of fine and reactive powders: phosphate dicalcium dihydrate, calcium dihydroxide, and βTCP (percentage of 5 % wt, granule seize <100 µm). The highly porous βTCP granules (percentage of 20% wt, granule size from 200 to 500 µm with 85% vol porosity) were finely mixed with the viscous past. The organic additives are added to the cement formulation to control the setting times and promote the cohesion and malleability of the past.

The fresh composite cement was molded in spherical form and immersed in deionized water at 37 °C for physico-chemical and morphological characterization. The results show that the cement set in a relatively short time (5-30 min) and the end-product sample consisted in 24 h of formed nanoapatite phase and unreacted βTCP granules. The fine TCP powder contributes actively to the rapid formation of apatite conferring a good mechanical stability of hard sample. Immersion in an acidic solution of hardened cement leads to the dissolution of βTCP phase offering the formation of the pores confirmed by X ray diffraction and microscopy.

The use of nano–β TCP powder and porous βTCP granules can significantly make our cement usable as a bioactive and bioabsorbable biomaterial favorable to good orthopedic and dental applications.

Key words: Cement, apatite, β-tricalcium phosphate, porous granules, dissolution.

C.A. 35

Experimental study of cement clinker modified under the effect of gypsum types by electrochemical impedance spectroscopy

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The recovery of industrial waste, in general, falls largely within the field of civil engineering of construction of cement-based materials, since they are basic materials [1]. In this study, electrochemical impedance spectroscopy tests and compressive strength tests were used to study the influence of gypsum types on a modified clinker cement paste, and the law of change of spectrum electrochemical impedance as a function of gypsum type was analyzed. Based on the typical equivalent circuit model of cement-based materials and its microstructure equivalent circuit model, the change law of electrochemical parameters and its relationship with compressive strength were analyzed. The experimental results (XRD, Compressive strength and TGA-DTA) indicate the influence that with different types of gypsum.

Keywords: Cement, Clinker, Gypsum, Paste, Compressive strength, Impedance.

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C.A. 36

Optimization and effect of different parameters on the compressive strength of fly ash geopolymer using the Box-Behnken Design

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This scientific article explores the optimization of fly ash geopolymer preparation conditions and presents a comprehensive physicochemical characterization of the resulting materials. Geopolymers, known for their sustainable and high-performance properties, are synthesized through a careful study of raw material selection, alkaline activator concentration, curing conditions, and post-curing treatments. The study evaluates the influence of these parameters on the geopolymerization process and aims to identify the optimal conditions for improved material properties. In parallel, advanced testing methods, including analytical techniques to characterize the structure, composition, and morphology of geopolymer materials, and mechanical strength assessment, provide insight into the structure-property relationships within the geopolymer matrices. The integration of Behnken box design (BBD) and detailed characterization techniques contributes to a deeper understanding of the geopolymerization process and facilitates the design of geopolymers with tailored properties for various applications. The results presented here have implications for the advancement of sustainable construction materials and the promotion of innovation in the field of geopolymer technology.

Keywords: Geopolymer, Optimization, Box-Behnken Design, Mechanical resistance, Fly ash

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C.A. 37

New Nanometric Lamellar NaxCoO_2 Synthesis Route Based on Solution Combustion (SC) of Cellulose Metal Organic Framework (Cell-MOF): Synthesis and Stoichiometry

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In this paper, we elaborate new Nanometric Lamellar NaxCoO_2 using a new synthesis method based on biodegradable cellulose based derivatives. The process of metallic ions complexation was studied using molecular dynamics (MD) simulations were performed to light up the optimized chemical system. The phase was confirmed successfully using structural analysis (FTIR, TGA/DTA, XRD, ICP, SEM and Raman).

Keywords: molecular dynamics (MD), cellulose, NaCoO2.

C.A. 38

Electrospinning Immobilization of Probiotics in Polymer Nanofibers

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The immobilization of probiotics in dry form preserving their activities, is important for many applications. The objective of this work is to apply an alternative to conventional immobilization techniques, using the nano-encapsulation of probiotics in nanofibers developed by Electrospinning as a new promising method.

In this study, the encapsulation parameters of probiotics were optimized while varying the electrospinning parameters. The mixture of polyvinyl alcohol and sodium alginate (PVA/SA) was used as an encapsulation material for the Lactobacillus paracasei strain due to their biocompatibility, their non-toxicity and their good chemical and thermal stabilization. A bacterium-free control film was prepared under the same conditions. The morphological and molecular characteristics of the developed nanofibers were studied by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FITR). In addition, a viability test and a molecular identification, by sequencing the 16S rDNA of the encapsulated strain were carried out to evaluate respectively the viability of the strain and the success of the encapsulation process.

SEM observations of the prepared films, have clearly shown that the nanofibers electrospinned from the mixture of Polyvinyl alcohol, Sodium Alginate and Lactobacillus paracasei have a uniform well defined and smooth structure, with beads of different lengths between 842 and 1000 nm.The diameter of the nanofibers, the molecular and morphological analyses of this study confirmed the encapsulation of Lactobacillus paracasei in polymer-based nanofibers. In view of these results, electrospinning represents a potential method for the incorporation of probiotics into solid administration systems.

Key words : Electrospinning, Nano-encapsulation, Biopolymers Nanofibers, Probiotic.

C.A. 39

Elaboration of antibacterial and antifungal Polyacrylic Acid films using solvent casting method

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Polyacrylic acid films have received considerable attention due to their versatile applications in various fields. In this study, we present a novel approach to fabricate polyacrylic acid films with improved antibacterial properties using the solvent casting method. The incorporation of glycerol as a plasticizer further improves the mechanical properties and flexibility of the film.

Various concentrations of antibacterial agents were introduced to functionalize the films and impart novel characteristics. The films were subjected to diverse analytical techniques, including scanning electron microscopy (SEM), Fourier Transform Infrared (FT-IR), thermogravimetric analysis (TGA), as well as tensile and elongation tests. This comprehensive analysis aimed to characterize the films and assess their mechanical, physical, and chemical properties. The antibacterial and antifungal activities of the films were rigorously tested to validate their potential as intelligent antibacterial films. The resulting films exhibited notable attributes such as flexibility, transparency, and exceptional antibacterial efficacy. These findings open avenues for the development of alternative antibacterial films for biomedical applications, presenting opportunities to replace synthetic counterparts with materials that showcase promising properties.

Keywords: polyacrylic acid, antibacterial, antifungal, solvent casting.

C.A. 40

Hybrid Polyvinyl Alcohol-Silica Antibacterial Nanofiber Fabricated by Combined Sol-Gel and Electrospinning Techniques

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Organic-inorganic hybrids are important in many fields because they combine the desirable properties of inorganic and organic phases. In this work, Polymer-silica hybrids Nano fiber with excellent antibacterial properties were synthesized using silica and polyvinyl alcohol (PVA) through a combination of sol-gel and electrospinning methods. The nanofibers, incorporating chloropropyltriethoxysilane (CPTS), PVA, and benzalkonium chloride as an antibacterial agent, were analyzed for their morphology, chemical composition, mechanical, thermal properties, and antibacterial activity. Results indicate that factors like polymer concentration significantly influence the fibers' formation and properties. Nanofiber prepared with 8% PVA solution, showed optimal characteristics in terms of fibrous structure, mechanical strength, and antibacterial efficiency. This study highlights the potential of electrospinning in developing advanced hybrid nanofibers with diverse applications.

Keywords: Electrospinning; Hybrid; Nanofiber; Sol-gel; Antibacterial, Polyvinyl alcohol; Silica.

C. A. 41

Advanced eco-friendly nanoporous macro-hierarchical nanofibers made from α-chito-protein with exceptional efficiency in removing dyes from aqueous environment

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A chitin complex derived from natural shell was tested for its ability to biosorb two inexpensive dyes: Acid Red 337 (AR) and the 1:2 chromic complex of Acid Blue 349 (AB). Factors considered included biosorbent characteristics, dye concentration, contact time and working pH. SEM images of the biosorbent show different morphologies and pore structures. FTIR, DRX, XPS and BET of the biosorbent shows the presence of the nanoporous complex α-chito-protein with a macro-hierarchical structure. Biosorption of the AR dye is higher than that of the AB dye for all sorbents. Outstanding biosorption capacity for red and blue acids, with maximum adsorption capacities in excess of 160.99 mg/g. Adsorption kinetics obey the pseudo-second-order model. The Freundlich model best matches experimental sorption isotherms. Thanks to these processes, we have been able to clean up industrial wastewater and prove the value of chitin as an effective biopolymer in a number of fields of application. Chemical preparation and functionalization methods, as well as characterization techniques, have enabled us to solve this problem successfully. The current study suggests that the sorbent derived from the wastes studied is effective in removing low-molecular-weight acid dyes from water.

Keywords: biomaterial, nanoporous, biosorption, anionic dyes, chitin, kinetic isotherm.

C.A. 42

Development of novel nano-materials type ABO_3 for Photocatalytic application

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The aim of this project is to study the influence of co-substitution of Sr by A ions and Ti by B ions in $SrTiO_3$ type perovskite. The effect of the substitution was investigated on it's structural, optical and magnetic properties at room temperature. $Sr_{1-x}A_xTi_{1-x}B_xO_3$ (x = 0, 0.6, 0.8 and 1) nanocrystalline have been prepared by solid state reaction. X-Ray diffraction, UV-Visible spectroscopy, and Superconducting quantum interface device (SQUID) magnetometer MPMS (Magnetic Property Measurement System) studies of $Sr_{1-x}A_xTi_{1-x}B_xO_3$ with (x = 0, 0.6, 0.8 and 1) perovskite compounds were carried out. Rietveld refinement showed that one phase transition occurred as a function of increased A and B contents; from cubic to orthorhombic structure. The band gap energy decreases from 3.25 eV to 2 eV with increasing A and B ions. The lattice distortion has profound effect on magnetic property which a strong ferromagnetic behavior of $Sr_{1-x}A_xTi_{1-x}B_xO_3$ with (x = 0.6 and 0.8) was observed.

Keywords: $Sr_{1-x}A_xTi_{1-x}B_xO_3$ perovskite oxide; X-Ray Diffraction; Rietveld refinement; UV-Visible spectroscopy; solid state reaction; band gap Energy; Ferromagnetism.

C.A. 43

Innovative Nanocomposite Utilising Metal-Organic Framework and N-Doped Biochar from Anaerobic Digestion By-Product: Advancing Adsorption and Peroxydisulfate Activation for Organic Pollutant Removal in Water

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A novel nanocomposite comprising Metal-organic framework (MOF) integrated with N-doped biochar (N-BC) was synthesized and applied for the removal of various emerging contaminants, including Reactive Black 5 (RB5), Sulfamethoxazole (SMX), and Cefazoline (CFZ). In this study, MOF prepared using hydrothermal technique at 110°C for 20h, while nitrogen-doped biochar (N-BC) was obtained through pyrolysis at 800°C in 3h of a blend of sewage sludge digestate (SSD) and urea, serving as a nitrogen source to eliminate targeted organic pollutants by synergistically employing adsorption and heterogeneous degradation via potassium peroxydisulfate activation. The impact of different SSD/urea ratios (1:0, 1:1, 1:3, 1:6, 1:9) on the performance of organic pollutant elimination was meticulously examined. The optimal ratio for N-BC preparation was determined to be 1:3, which was subsequently combined with MOF to create the nanocomposite. Various characterization techniques were employed for comprehensive textural, morphological, and structural analyses. Experimental results demonstrated exceptional efficiency of the prepared nanocomposite in both adsorption and degradation of targeted contaminants, with MOF serving as the adsorbent and N-BC playing a crucial role in pollutant degradation via peroxydisulfate activation.

Keywords: Metal-organic framework, N-doped biochar, Adsorption, Peroxydisulfate activation, Wastewater treatment.

C.A. 44

Preparation and characterization of ecological nano-pigments based on rare earth phosphates

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Inorganic pigments are supported by a long history. These pigments are widely used to cover and color tools and materials that work in with range of temperature [1]. Today, nano-pigments play an important role in industry [2]. There are numerous researchers that one cried out to synthesis environmentally friendly pigments [3,4].

In this sense, we synthesized a new set of rare earth phosphate nano-pigments by hydrothermal method followed by calcination. These phosphate compounds Ce0.2Bi0.8PO4, $Nd_{0.3}Bi_{0.7}PO_4$ and $Ca_{0.2}Er_{0.8}PO_4$ were calcined at 900 °C for 4 hours, by observing the formation of three pigments of different colorations: green, purple and orange. The final nanopowders were characterized by X-ray diffraction (XRD), Fourier Transform Infrared (FT-IR) and Raman spectroscopy.

The pigments synthesized showed thermal stability and the presence only of the orthophosphate group in these matrices. The final colors were evaluated according to the CIE-1976 L^* a^* b^* method by obtaining a standard identification of each color. The coloring qualities and thermal stability of these prepared samples indicate that these materials can potentially be used as naturally occurring environmentally friendly pigments in paints and plastics.

Keywords: Rare earth phosphate, nano-pigments and environmentally friendly pigments

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C. A. 45

New mercury (II) coordination frameworks involving tetrazole ligand formed in situ: Synthesis, spectroscopic characterization and crystal structure

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Over the past decade, significant advancements in porous materials, particularly Metal–Organic Frameworks (MOFs), have been notable due to their diverse applications such as gas storage, separation, catalysis, nanomaterials, and coordination chemistry. Concurrently, the chemistry of d^{10} metal ions, specifically Hg^{2+}, Cd^{2+}, and Zn^{2+}, has garnered considerable attention owing to their ability to construct 1D, 2D, and 3D polymeric networks with advantageous physical and chemical properties relevant to energy, biology, and magnetism. The selection of metal ions and organic ligands plays a pivotal role in determining the resulting architecture and properties of these materials, with recent focus on heterocyclic compounds derived from the tetrazole family. Tetrazole molecules, characterized by their high nitrogen content and diverse substituents, offer versatility in forming various complexes and polymers with different transition metals. Synthesis of tetrazole ligands often includes a (3+2) dipolar cycloaddition between azide and acetonitrile. Herein, we present the synthesis and characterization of a novel coordination complex involving in situ tetrazole ligand with the transition metal Hg(II). The synthetized complex has been fully characterized by single crystal X-ray diffraction, UV-Visible, as well as FTIR spectroscopy. Single-crystal X-ray diffraction analysis reveals the compound to be a MOF type, $[Hg(Mtz)_2]$ (Mtz = Methyl tetrazole), crystallizing in the triclinic P-1 space group. The asymmetric unit contains two mercury Hg(II) atoms, each coordinated to four molecules of 5-methyl tetrazole. The resulting polymeric structure exhibits a MOF topology, with Hg(II) metal centers serving as four-connection nodes and methyl-tetrazole (Mtz) acting as an organic connector bridge. The spectroscopic characterization is also described and discussed.

Keywords: MOF_S; Tetrazole; Mercury; Coordination complex; Crystal structure.

C. A. 46

Extraction of a natural indigo blue pigment from the *Isatis tinctoria L.* plant and dyeing of cotton fabrics

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The fresh leaves of *Isatis tinctoria L.* have been exploited in indigo production to optimize the dye's yield and guarantee its quality through various extraction methods. This study begins by exploring the structure and properties of indigo, the extraction of vegetable indigo from woad, and a comparison with the synthetic method, examining its advantages and disadvantages. The main aim is to improve the efficiency of indigo extraction, using an environmentally friendly approach, while developing a rapid and reliable process for assessing indigo yield. To verify the structure of the indigo obtained, data from the literature were used to develop methods for the quantitative analysis of natural indigo. Three previously prepared samples of blue indigo powder were applied to cotton fibers for dyeing, optimizing the dyeing procedure and examining the factors influencing it. Analyses such as UV-visible spectroscopy were carried out to characterize the samples, followed by infrared spectroscopic analysis to identify functional groups. Color intensity was measured using a colorimetric data spectrophotometer.

Keywords: Indigo, extraction, cotton, *Isatis tinctoria L.*

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C. A. 47

Structure, Infrared, Raman spectroscopic and optical study of orthophosphates $BaM_{0.5}Nb_{0.5}(PO_4)_2$ with M trivalent cation

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Phosphates with general $A^{II}M^{IV}(PO_4)_2$ formula crystallizing in several structural types as Monazite, Zircon (Xenotime), Scheelite, Cheralite and Yavapaiite [1-3]. The synthesis and structural study of $Ba(Nb^{V}_{0.5}Fe^{III}_{0.5})(PO_4)_2$ phosphate belonging to the Ba-Nb-Fe-P-O system were reported here for the first time. Structure of $Ba(Nb^{V}_{0.5}Al^{III}_{0.5})(PO_4)_2$ obtained by solid state reaction in air atmosphere, were determined at room temperature from X-ray powder diffraction using the Rietveld method. $Ba^{II}(Nb^{V}_{0.5}Fe^{III}_{0.5})(PO_4)_2$ Results show that $Ba(Nb_{0.5}Fe_{0.5})(PO_4)_2$ crystallize in monoclinic *C2/m* space group (Z = 2) with cell parameters a = 8.295(5) Å; b = 5.165(4) Å; c = 7.734(3) Å and β = 93.890(1)°. Raman and Infrared spectroscopic study were used to obtain further structural information about the nature of bonding. The UV-visible properties showed indirect optical gap energies 3.51 eV.

Keywords: Iron phosphate, Monazite structure, X-ray powder diffraction, Rietveld method, UV-visible

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C. A. 48

The Synthesis and Comprehensive Analysis of $Co_2P_2O_7$ Compound: A Study of Its Properties and Characteristics

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The synthesis of nanomaterials and especially nanoparticles has been of increasing interest in the last decades[1-2]. The purpose of this work is to develop, by solid and citrate state, structural and morphological characterization of $Co_2P_2O_7$. The first process is the most used solid-state reaction technique starting from three materials: CoO, and $(NH_4)_2HPO_4$ with the appropriate amounts. The second method involves the reaction of metallic chlorides and $(NH_4)_2HPO_4$ using citric acid as a complexing agent. The phosphate $Co_2P_2O_7$ can be indexed within the P21/c space group indicating a monoclinic distortion3. The analysis by DRX, FTIR of double $Co_2P_2O_7$ indicate the presence of a single phase. The powder particles obtained have a heterogeneity of microstructure.

Keyword: Citrate pathway; Solide state, Characterization; $Co_2P_2O_7$; Morphology.

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C. A. 49

Structural and optical characterization of newly synthesized $BaSb_xCr_xTi_{1-2x}(PO4)_2$ yavapaiite phase

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A series of yavapaiite-type phosphates $BaSb_xCr_xTi_{1-2x}(PO_4)_2$ ($0 \leq x \leq 0.5$) has been synthesized by solid-state reaction. The crystal structures were characterized by X-ray diffraction and Rietveld refinement. The compounds crystallize in the monoclinic system with space group C2/m. The effects of substituting titanium with antimony and chromium on the lattice parameters, bond lengths, and angles were investigated. The vibrational properties were examined by infrared spectroscopy. The IR spectra revealed characteristic bands of the PO_4^{3-} tetrahedra. The UV-visible absorption spectra showed the influence of Sb/Cr substitution on the optical band gap. Direct band gap values in the range of 1.3-2.1 eV were obtained, indicating semi-conducting behavior. The results demonstrate that partial replacement of Ti^{4+} by Sb^{5+}/Cr^{3+} impacts the structural and optical properties of the $BaSb_xCr_xTi_{1-2x}(PO_4)_2$ phosphates. The optical band gap can be tuned by adjusting the Sb/Cr content.

Keywords: Rietveld Refinements analysis, X-ray powder diffraction, yavapaiite structure, IR spectroscopy, UV-visible and band gap.

C. A. 50

Hydrothermal Synthesis and Crystal Structure of a Novel Phosphate: $CdMn_4(HPO_4)_2(PO_4)_2.4H_2O$

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The new cadmium and manganese-based phosphate $CdMn_4(HPO_4)_2(PO_4)_2.4H_2O$, was synthesized by a hydrothermal method and its structure investigated by single crystal X-ray diffraction. The accuracy of the resulting structural model was verified using the Bond-Valence-Sum (BVS) and Charge-Distribution (CD) methods. This phase is a new member of the Hureaulite family and crystallizes within the monoclinic system (space group C2/c, a = 17.6932(5) Å, b = 9.1862(3) Å, c = 9.5417(3) Å, β = 96.562(1)°, and Z = 4). In this crystal structure the metal cations are statically distributed over three independent sites. The first two are located at the general position 8f and are entirely filled by $Cd(1)^{2+}/Mn(1)^{2+}$ and $Cd(3)^{2+}/Mn(3)^{2+}$ while the remaining site is situated at the special position 4e(2) and fully occupied by $Cd(2)^{2+}/Mn(2)^{2+}$. The main structural groups of the asymmetric unit consist of three distorted $[(Cd(1)/Mn(1))O_5(OH_2)]$, $[(Cd(2)/Mn(2))O_6]$ and $[(Cd(3)/Mn(3))O_4(OH_2)_2]$ octahedra with two regular PO_4 & HPO_4 tetrahedra. The 3D-structure is made up of five sequential octahedral $(Cd/Mn)_5O_{16}(OH_2)_6$ units of edge-sharing running along the [001] direction. The connecting PO_4 and HPO_4 groups bind the interconnected units to one another by corners-sharing to create a 3D-framework defining a sizable void along the [001] direction hosting some H_2O molecules.

Keywords

Crystal structure, X-ray diffraction, Hureaulite, Hydrothermal synthesis

C. A. 51

Development and Characterization of Novel Phosphate Glass system through the Incorporation of Natural Phosphate

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Phosphate glasses were produced through the incorporation of naturally occurring phosphate into a glass matrix. The synthesis process involved the use of the standard melt- quench method, Analysis of the X-ray diffraction (XRD) patterns indicated that all the samples exhibited an amorphous feature, suggesting the absence of any long-range ordering in the atomic arrangement. This finding has been further supported by the Differential Scanning Calorimetry (DSC) analysis results, assessing the glassy nature of the samples and allowing the study of the thermal parameters as well as the thermal stability of the as-prepared glasses. The variation of both density and molar weight have been explored and discussed. Additionally, the molecular structure of the glasses has been investigated using the Fourier Transform Infrared Spectroscopy (FTIR) and Raman spectroscopy. The obtained results revealed that P_2O_5 acted as a network former contributing to the establishment of a vitreous network. Moreover, it has been observed that the presence of P_2O_5 facilitated the formation of metaphosphates and pyrophosphates groups. Furthermore, the formed crystalline phases upon the annealing process have been identified and discussed.

Keywords: Phosphate glasses; Natural Phosphate; XRD; DSC; FTIR; Raman.

C. A. 52

Efficient Methylene Blue Adsorption Using a bio-adsorbant Hydroxyapatite-AMP Composite

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The research examined the removal of methylene blue (MB), a prevalent cationic dye, from water using a new composite material made by combining hydroxyapatite (HAp) with aminotrimethylphosphonate (AMP), referred to as HAp-AMP. This composite was created through a simple and economical process that leverages the intrinsic qualities of HAp and AMP's ability to modify surfaces. The objective was to assess the adsorption capability of HAp-AMP in purifying water by eliminating MB. Various analytical methods, such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and Brunauer-Emmett-Teller (BET) analysis, were employed to characterize the HAp-AMP composite, confirming its successful formation with distinct structure and improved surface characteristics.

In the study, batch adsorption tests were performed to determine how various factors like initial MB concentration and contact time affect the adsorption process. These tests, along with the application of kinetic and isotherm models, helped clarify the adsorption mechanisms and identify the best conditions for MB removal. The adsorption was found to follow a pseudo-second-order kinetic model, indicating a chemisorption process, and fit well with the Freundlich isotherm model. Additionally, the impact of the solution's pH on adsorption efficiency was explored, showing that HAp-AMP's adsorption capacity varied with the electrostatic interactions between MB and the composite, particularly favoring acidic conditions.

In summary, the HAp-AMP composite exhibited effective adsorption properties for extracting methylene blue from water, offering a valuable contribution to developing efficient and eco-friendly adsorbents for cleaning dye-polluted water, thus supporting environmental cleanup and water treatment efforts.

Keywords: Hydroxyapatite-AMP, novelbio-adsorbant, methylene blue, sustainable adsorbents, water purification

C. A. 53

Synthesis and characterization of Na-bentonite/hydroxyapatite composite

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Recently, composites based on hydroxyapatite and clay have been used in many fields, such as biomedical as a bone substitute [1, 2], environmental as an adsorbent [3, 4] and as catalyst [5]. In this study, a composite (Na-Bentonite/HAP) based on hydroxyapatite (HAP) and sodium-activated bentonite (Na-Bentonite) was synthesized by the neutralization method. The bentonite used in this study is very abundant clay in the Oriental Region of Morocco, consisting mainly of the montmorillonite (MMT). Na-Bentonite/HAP, HAP and bentonite were characterized by Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) coupled with Energy Dispersive X-ray Emission Spectrometry (EDX). The results of the XRD analysis showed the presence of characteristic peaks of both the MMT and the HAP, also indicating the formation of the HAP on the surface of the MMT. The IR spectrum of the composite (Na-Bentonite/HAP) showed the presence of adsorption bands characteristic of Hap corresponding to the phosphate (PO_4^{3-}), hydroxyl (OH^-) and chemical bonds Si-O, Al-O that characterize the montmorillonite. SEM observations revealed that the presence of HAP has caused the agglomeration of MMT particles. EDX analysis showed a Ca/P molar ratio of 1.61, corresponding to a calcium-deficient hydroxyapatite.

Keywords: Composite, hydroxyapatite, bentonite, montmorillonite.

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C.A. 54

Deciphering the Magnetic Enigma of Water: Investigating its Influence on Diammonium Phosphate (DAP) Fertilizer Solubility

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In the field of agriculture, fertilization stands as a pivotal technique. Diammonium phosphate (DAP) holds wide popularity for enriching soil with nutrients. The degree of DAP 's solubility in water assumes a critical role in determining its effectiveness for fertigation. Our research delved into three key experimental variables: the quantity of DAP, the duration of magnetization, and the type of water, all with the objective of optimizing these factors to maximize Total Dissolved Solids (TDS). Leveraging Minitab software, we harnessed a comprehensive factorial model comprising nine experiments (3x3). Our investigation unveiled that TDS was notably influenced by the type of water, closely followed by magnetization duration and DAP content. Water type contributed the most significantly at 56.16%, followed by DAP content at 40%, and magnetization time (tm) at 3.86%. The ideal combination of factors for achieving an elevated TDS value was pinpointed at 8% DAP content, 10 minutes of water magnetization, and the utilization of saline water (SW). These research findings have the potential to inspire farmers to embrace environmentally sustainable fertigation practices in their agricultural management.

Keywords: TDS, Minitab, Diammonium phosphate, Magnetized water, DAP

C. A. 55

Synthesis, Characterization and Structural Study of the Novel Phosphate $Ag_{0.4}Zn_{2.8}Fe_4(PO_4)_6$

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$Ag_{0.4}Zn_{2.8}Fe_4(PO_4)_6$ was prepared by classical solid-state method and investigated by means of single-crystal X-ray diffraction (XRD). The purity of the sample was checked by energy dispersive X-ray spectroscopy (EDS). This new phase adopts the typical Howardevansite structure with the triclinic system, space group P-1 and unit cell parameters: a = 6.3551(1), b = 7.9271(1), c = 9.3232(2) Å, α = 105.022(1)°, β =108.085(1)°, and γ = 101.470(1)°. All atoms of the crystal structure occupy the general position 2i except $Ag(1)^+$ and $Zn(1)^{2+}$ cations which are on two centers of inversion at 1g(-1) and 1h(-1), respectively. This crystal net-framework is made up of folded chains of polyhedral with shared edges based on $[Fe(1)_2 O_{10}]$ and $[Fe(2)_2 O_{10}]$ dimers intercalated by $Zn(2)O_5$ unit. Adjacent chains are interconnected by a regular PO_4^{3-} tetrahedra and ordered in stacked layers perpendicular to [010]. Such an arrangement gives rise to tunnels parallel to [100], that host $Ag(1)^+$ and $Zn(1)^{2+}$ cations. The stability and accuracy of the suggested structural model have been approved by combinatorial investigations of charge distribution (CD) and bond valence sum (BVS).

Keywords: Solide-state reaction, Howardevansite, Phosphate, Crystal structure

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C. A. 56

Development of Tricalcium Phosphate-Chitosan composite beads: towards high crushing strength for bone repair

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In the field of bone tissue engineering, there has been a notable increase in demand for the creation of biocompatible materials specifically designed for bone repair purposes. In response to this demand, our study introduces a biocompatible composite material, prepared from calcium phosphate (TCP) and chitosan, fashioned into beads for versatility in size, texture, and firmness. The TCP synthesis followed the neutralization method outlined by Elouahli et al. [1], while chitosan preparation and characterization protocols were detailed by Derraz et al. [2]. The TCP/Chitosan composite was synthesized by incorporating TCP into the chitosan solution at varied percentages (10%, 20%, and 30% chitosan). the obtained slurries were used to fashioned spherical beads of the composite. Subsequently, the obtained beads undergo scrutiny via XRD, FTIR, and TEM techniques, with hardness gauged through crushing force assessments.

The results highlight the superiority of the composite TCP-30CS, with a composition of 70% apatitic tricalcium phosphate and 30% chitosan, dried at 37°C. In fact, this composite formulates exhibited the highest crushing strength that reached 4.25 Kg.f. These findings suggest promising applications of these bio-composite as bone repair in tissue engineering.

Keywords: composite, bone tissue repair, chitosan, tricalcium phosphate (TCP), beads, neutralization method

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C.A. 57

Phosphate-based Biomaterials as Carriers for Antibiotics for Local Treatment of Bone Infection

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Bone infection is a major public health issue. Numerous studies have reported thelimitations of systemic antibiotherapy for bone infection, such as the insufficient vascular supply, the occurrence of side effects, and the development of microbial resistance to antibiotics (Amiri et al., 2020). Alternatively, local treatment of bone pathologies is an innovative strategy. It can compensate for systemic therapy-associated limitations by delivering the therapeutic agent in situ, thereby limiting the occurrence of adverse effects and drug resistance (Sadowska et al., 2021). The association of antibiotics with calcium phosphates-based biocomposites for the local treatment of bone pathologies has received increasing interest in orthopaedics (Chen et al., 2021). Therefore, the comprehension of the involved mechanisms is crucial for the development of controlled drug-release systems, and the determination of their performance in vitro and in vivo. Accordingly, the adsorption approach is a key step as it can shed light on the driving forces in the drug's retention and release phenomena with phosphate compounds. Here, we aim to study the adsorption of an antistaphylococcal drug onto phosphate compounds, and to elucidate their mode of interaction. The adsorption kinetic and isotherm performed at physiological pH indicated a fast uptake process of the antibiotic and an uptake amount in the range of 22 to 62 µg/g. The evolution of the loading capacity of the drug was correlated to the intrinsic physicochemical properties of the investigated sorbents. The formulated composites exhibit promising properties for application in targeted treatment of bone-associated infections.

Keywords

Bone infection, Antibiotic, Calcium phosphates, Adsorption, Drug-delivery

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C.A. 58

Valorization of Phosphate sludge by HCl attack

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c OCP Group

Phosphate scrubbing sludge are very fine particles that forms during the process of enriching phosphate ore. Phosphorus is separated from the gangue minerals by a combination of different processing units; grinding, screening, washing and flotation. It is during the penultimate operation that the phosphate sludge is generated.

These sludge, which contain some level of P_2O_5 and high carbonate content, are stored in tailings ponds, generally in the open air and eventually form dikes that disfigure the landscape and arable land and harms the natural development of fauna and flora.

In this study, experiments have been carried out to reduce carbonate content by leaching sludge with dilute hydrochloric acid solution. Effects of hydrochloric acid concentration, reaction time, temperature and liquid/solid ratio (vol./wt. basis) on the process have been studied. Under the reaction conditions, sludge are dissolved to form soluble Monocalcium Phosphate during the selective leaching.

Lime milk is used to recover the dissolved sludge and produce Dicalcium Phosphate (DCP). P_2O_5 content can be raised up to the industrially acceptable level due to the selective reduction/elimination of calcium carbonate content of sludge, depending on the reaction conditions as well as nature and size of sludge's particles.

C.A. 59

Préparation d’un nouveau catalyseur stable et régénérable à base des schistes bitumineux: Application à la synthèse des imines

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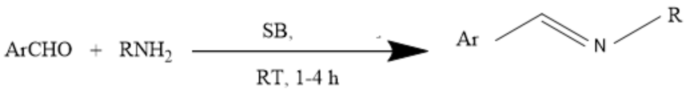
Les schistes bitumineux représentent une richesse minière naturelle pour le Maroc. A ce titre, il représente un enjeu stratégique national pour les développer dans plusieurs domaines surtout dans le secteur énergétique. Ce sont des roches sédimentaires possédant une matrice organique et une matrice minérale.

De nombreuses études [1,2] ont été consacrées pour développer les schistes bitumineux marocains surtout l’exploitation pour la production de l’énergie par combustion directe dans des centrales électriques, ou bien par la pyrolyse pour produire des huiles à partir les roches de schistes.

Le défi et l’objectif primordial fixés actuellement par les différentes équipes de recherche dans le domaine de la catalyse hétérogène résident dans l’obtention des rendements élevés avec une excellente sélectivité et une bonne application aux conditions expérimentales douces illustrant les concepts de la chimie verte. Pour cela, nous nous sommes intéressés à élargir le domaine d’application de schiste bitumineux par son utilisation dans le domaine de la catalyse.

Ce travail a pour objectif d’élaborer un nouveau catalyseur hétérogène, stable et régénérable à base de schiste bitumineux (**SB**) et son utilisation dans la synthèse des imines à partir des aldéhydes aromatiques et différentes amines (schéma).



Mots clés : Schiste bitumineux, imines, matériau stable, catalyse hétérogène

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C. A. 60

Schistes bitumineux marocains : nouveaux catalyseurs stables et régénérables pour la réaction de protection des aldéhydes aromatiques par l'anhydride acétique

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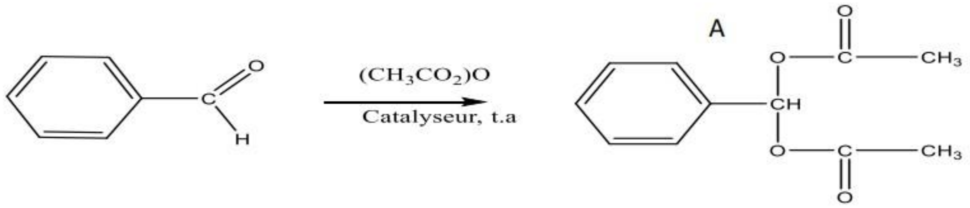
La protection des groupes carbonyles joue un rôle important dans la synthèse organique multi- étapes des produits naturels complexes. La protection des aldéhydes sous forme d'acylals, d'acétals ou de dithioacétals est l'une des transformations plus importantes au cours de la synthèse multi-étapes. De nombreuses méthodes sont disponibles pour la synthèse de 1,1-diacétates à partir d'aldéhydes et d'anhydride acétique. Bien que certaines de ces méthodes offrent un rendement plus élevé de diacétates correspondants, la majorité souffre d'un ou plusieurs inconvénients tels que des conditions acides dures, de longs temps de réaction, le besoin d'un catalyseur coûteux et une quantité stœchiométrique ou excessive de réactifs [3].

Dans ce travail, nous avons élaboré un nouveau catalyseur hétérogène, stable et régénérable à base de schiste bitumineux (**SB**) et nous l'avons utilisé dans la protection des aldéhydes aromatiques par l'anhydride acétique (schéma).



Mots clés : Schiste bitumineux, aldéhydes, amines, matériau stable, catalyse hétérogène.

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C. A. 61

Adsorption of the crystal violet dye on an adsorbent material prepared from Moroccan oil shales

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This work aimed to elaborate and characterize materials prepared from the Moroccan oil shales of the Timahdit region (layer X) and their use for the removal of the crystal violet dye (CVD) from aqueous solutions. The adsorbent material, referred to as XHA, was characterized by Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM), coupled with EDS analysis. It was then used for the adsorption of the CVD in a batch system. This process was highly dependent on the physico-chemical parameters, such as the solution pH, the temperature, the contact time, and the CVD initial concentration. The elimination of CVD by XHA reached 98.75 %, and the process kinetic was of pseudo-second order. The adsorption capacity was 19.75 mg/g, according to the Langmuir model. The thermodynamic studies indicated that dye adsorption by XHA is spontaneous, endothermic, and of physisorption nature.

Keywords: Adsorption, Oil shale, Cristal violet dye, Adsorption isotherm, Thermodynamic parameters

C. A. 62

Adsorption of Ciprofloxacin antibiotic on materials prepared from Moroccan oil shales

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Ciprofloxacin antibiotic (CIP) adsorption was investigated using an adsorbent material (XHA) obtained by chemical activation using phosphoric acid (H_3PO_4) of Moroccan oil shales of the Timahdit region (layer X). The results obtained show that the adsorption process is highly dependent on the physicochemical parameters. The mechanism of CIP adsorption was better described by the kinetic model of the pseudo-second-order and obeyed both linear and non- linear models of the Langmuir isotherm. The maximum adsorption capacity is equal to 81.11 mg/g. Furthermore, the evaluation of thermodynamic parameters, such as free energy, enthalpy, and entropy suggested that the CIP adsorption on XHA is a spontaneous physisorption process with an exothermic effect.

Keywords: Oil shales, Adsorption, Ciprofloxacin, Adsorption kinetic, Isotherm analyses

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C. A. 63

Enhancing the energy potential of Tarfaya oil shale: investigation of decarbonation effect on pyrolysis thermal behavior.

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Morocco aims to reduce climate change and decrease reliance on fossil fuels through a comprehensive plan for net zero carbon emissions. By prioritizing renewable energy sources and reducing greenhouse gas emissions, Morocco is taking systematic steps to address both environmental challenges and energy dependency. Research suggests that oil shale, with its abundant fossil organic matter, holds significant energy potential, furthering Morocco's pursuit of alternative energy resources [1,2]. Nevertheless, the mineral composition of oil shale restricts its industrial exploitation in many countries. To fully exploit this resource, several innovative methods have been developed, including the use of hydrochloric acid to concentrate oil shale. In this study, an innovative method was developed to maximize the energy yield of oil shale using acetic acid to decarbonize the rock through green chemistry processes, thereby enhancing the industrial potential of this unconventional energy resource. Furthermore, treated oil shales can be exploited in various industrial applications such as CO2 absorption, benefiting from an increase in their porosity and specific surface thanks to the modification of their structure by acid attack, thus improving their capacity to adsorb greenhouse gases.

Herein, the main objective of this study is to investigate the effect of acetic acid decarbonation of oil shale from the Tarfaya deposit on the thermal behavior of the pyrolysis process, as well as to determine the relative kinetic parameters, based on mechanistic models. The results obtained confirmed the significant effect of oil shale decarbonation on the energy performance of oil shale concentrates, obtained after treating the rock with acetic acid under extremely mild conditions (low acid concentration and ambient temperature).

Keywords: Moroccan oil shale [1], decarbonization [2], pyrolysis[3], kinetic parameters [4]

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C. A. 64

Synergistic Enhancement of Pollutant Degradation through Adsorption and Photocatalysis using Different Raw-Clay based Nanocomposites: Preparation, Characterization, and Kinetic Study

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Our research aims to synthesize rapid and effective materials using various catalysts. We also investigate the effect of different binary metal oxides doping on the photocatalytic activity of the clay for dye degradation. The as-prepared nanocomposites were characterized using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscopy with Energy Dispersive X-ray (SEM/EDX). The obtained findings confirm the effective immobilization of the semiconductor onto the clay. The impact of contact time was assessed to elucidate the mechanisms involved in the adsorption and photodegradation processes of the dye by the nanocomposites. The dye removal reaches a significant percentage under UV irradiation. The kinetic data were in good agreement with the pseudo-second-order model. The overall outcomes of the experiments suggest that the newly developed material holds significant promise for effectively addressing water contamination issues caused by hazardous substances.

Keywords: Adsorption; Dye degradation; Semiconductor immobilized; Visible light photodegradation.

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C.A. 65

Characterization and alkali-activation of belitic clinkers from recycled materials

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The valorization of waste materials is linked to the development of a new construction material using waste materials with properties similar to ordinary Portland cement, which can be obtained by alkaline treatment. Three main operational parameters have been taken into account for the synthesis of this material: the liquid/solid ratio, the concentration in the alkaline solution and the activation temperature. The development of environmentally-friendly, energy-efficient building materials is a major concern for researchers, who are looking for simpler, more energy-efficient processes. As a result, the cement industry is experiencing a steady increase in the use of complementary materials, often of diverse origins. The aim of this study is to formulate and characterize belitic clinkers from recycled materials, replacing traditional raw materials, while examining the characteristics of the resulting phases. The phases activated with H_2O NaOH or KOH, using two different molarities (1M-3M), were analyzed in depth; the nature of the C-S-H in the hydrated products formed is examined after 7, 28 and 90 days, using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR).

Keywords: Dicalcium silicate, belitic clinker, alkali-activation, cements.

C.A. 66

Prétraitement de l'acide phosphorique industriel 29% en P_2O_5 : Rétention des métaux lourds par bentonite modifiée

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L'acide phosphorique produit par voie humide est riche en impuretés telles que les sulfates, le fluorure, les matières organiques et les métaux lourds. Ces impuretés, particulièrement les métaux lourds toxiques comme le cadmium, posent un défi important à la qualité de l'acide phosphorique industriel et à l'industrie des engrais. Des réglementations plus strictes limitent actuellement leur présence dans les engrais. A la lumière de travaux antérieurs déjà réalisés sur le prétraitement de l'acide phosphorique 29 % P_2O_5 par un matériau naturel [1-2], nous avons utilisé la bentonite brute et la bentonite activée et imprégnée de matériau sulfuré comme matériaux adsorbants à faible coût pour la rétention des ions métalliques lourds provenant de l'acide phosphorique brut 29 % P_2O_5.

L'analyse de l'argile bentonite collectée sur le gisement de Nador avant et après traitement d'activation et d'imprégnation est réalisée par plusieurs techniques physico-chimique (DRX, FX, IR et ATD-ATG) pour mettre en évidence l'effet ce traitement sur la bentonite naturelle.

Le prétraitement de l'acide phosphorique 29% en P_2O_5 par la bentonite naturelle et traitée est réalisé en régime statique selon un protocole simple, en tenant compte des facteurs qui peuvent influencer sur le traitement, à savoir : le temps de contact, la température et la masse de l'argile bentonite. La comparaison des résultats de l'analyse élémentaire par ICP-AES de l'acide, avant et après traitement, obtenus pour ces deux matériaux, montre une efficacité remarquable de la bentonite traitée pour la rétention des métaux lourds particulièrement le cuivre, le cadmium et le nickel en plus de de la matière organique et le fluor.

Mots clés : Phosphorique acide, Prétraitement, Bentonite, Adsorption, métaux lourds.

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C.A. 67

Adsorption of Methylene Blue Dye and Analysis of Two different moroccan Clays: Kinetics and Thermodynamics Study

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The purpose of this research was to learn more about the primary and secondary properties of two different Moroccan clay OC and RC in an effort to better investigate innovative adsorbents and gain access to an ideal adsorption system. The kinetics and isotherms experiments were also studied at different temperature. The results indicated that the methylene bleu adsorption reached equilibrium with in 2h30 h, and OC is the most effective clay for eliminating MB with an adsorption capacity of (79.61 $mg.g^{-1}$) greater than that of RC (67.79 $mg.g^{-1}$) .The two clays were characterized by various techniques (SEM/EDX, FTIR, X-ray fluorescence, DRX.). First- and second-order rate laws, representing two distinct kinetic models, were applied in the kinetic approach. Adsorption of dye MB onto natural clay was studied, and the results agreed with the 2-sec order model. The adsorption process was determined by applying the Langmuir and Freundlich isotherms and the thermodynamic parameters were calculated.

Keywords: Raw clay; Methylene Blue (MB) dye; Adsorption; kinetic and thermodynamic.

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C.A. 68

Eco-friendly insulation composite brick utilizing Coal Gangue, Fly Ash, and Marble Dust

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Rising concerns over environmental sustainability in construction have prompted a heightened focus on thermal insulation to reduce energy consumption. However, conventional approaches, particularly in brick manufacturing, contribute significantly to environmental degradation. To address these issues, this study introduces an approach to formulate porous brick with superior thermal properties by repurposing environmentally harmful materials, such as coal gangue, fly ash, and incorporating marble dust to enhance structural integrity. Three samples were prepared, varying the concentration of the activator solution, to investigate its impact on the structural characteristics of the bricks. Tests, including density, porosity, water absorption, mechanical strength, and thermal resistance, were conducted to assess the influence of the alkaline activator concentration on brick performance. The results revealed that increasing the concentration of sodium hydroxide (NaOH) led to a higher level of porosity in the samples, thereby enhancing thermal resistance. The thermal resistance reached 0.284 W/mK, accompanied by a moderate compressive strength of 2.73 MPa. The developed porous bricks are more heat-resistant than conventional clay bricks and Autoclaved Aerated Concrete (AAC) blocks. The improved thermal performance of these blocks not only offers energy efficiency benefits but also significantly reduces environmental impact.

Keywords: Coal gangue, Marble dust, Alkaline activator, Porosity, Thermal resistance, Mechanical strength.

C.A. 69

Utilisation des feuilles mortes de palmier pour l'amélioration des propriétés thermiques et mécaniques des briques de terre crue de la région de Goulmima

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L'intérêt grandissant pour les matériaux écologiques dans le domaine de la construction met en lumière leur rôle crucial pour une durabilité accrue. Cet article se penche sur l'exploitation des ressources naturelles de Goulmima, dans la région d'Errachidia, à travers l'étude des caractéristiques mécaniques et thermiques de briques de terre novatrices. L'originalité de ces briques réside dans l'incorporation d'un additif atypique : les feuilles de palmier séchées, résidu agricole largement disponible localement vu la sécheresse qui a touché notre royaume, en plus du grand changement des habitudes de la population de la région qui utilisait autrefois ces feuillies pour la cuisson et comme ajout dans les architectures en terre. Notre recherche évalue l'impact de cet additif végétal sur les qualités du matériau produit, visant à proposer une alternative durable et performante pour la construction. Par le biais d'analyses détaillées, nous explorons comment cette démarche écologique peut améliorer à la fois l'isolation thermique et la solidité des briques, proposant de nouvelles avenues pour l'emploi de matériaux renouvelables et locaux en construction.

Les briques conçues ont été caractérisées par plusieurs techniques : géotechniques (limites d'Atterberg, granulométrie …), physico-chimiques (DRX, IR, FX …) et microscopique (MEB). Les échantillons étudiés de plasticité moyenne sont formés d'argiles non gonflantes et du sable.

L'effet de l'ajout des feuilles mortes de palmier broyés sur les propriétés mécaniques, la conductivité thermique du matériau a été déterminé. La résistance à la compression des échantillons stabilisés a donné les meilleurs résultats pour un pourcentage de 3%. La conductivité thermique quant à elle, a révélé une diminution par rapport à l'échantillon de référence.

Mots clés : Terre crue, feuilles sèches de palmier, résistance à la compression, conductivité thermique.

C. A. 70

Utilizing Coal Gangue and Olive Pomace in the Elaboration of Fired Bricks

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In Morocco, the mining and oil industries produce many wastes, more than 20 million tons of coal gangue (CG) were accumulated in the abandoned mine of Jerada, meanwhile the production of olive oil generates 30% of a solid by-product called olive pomace (OP). These wastes pose an environmental problem directly affecting the ecosystems, thus the need to look for alternative ways to reduce their dangerousness, The aim of this study is to investigates the effect of using of CG and OP in the elaboration of fired bricks.

Samples were produced by mixing different weight percentages of OP (0%, 5%, 10%, and 15%) with CG, then sintered at 1050°C. The mixtures were characterized by X-ray diffraction and Fourier transform infrared spectroscopy. Bulk density, apparent porosity, water absorption, loss on ignition, compressive strength and thermal conductivity were measured to determine their physical, mechanical, and thermal properties. The results indicate that the addition of OP to CG has no effect in the fired bricks composition, but it led to a reduction in bulk density, compressive strength and thermal conductivity while causing an increase in apparent porosity loss on ignition and water absorption.

The addition of 15 wt% of OP, produced bricks with a compressive strength of 14.19 MPa, meeting the standards for clay masonry units. Concurrently, it improves thermal insulation by reducing thermal conductivity by 16.89% compared to the sample containing only CG.

Keywords: coal gangue, olive pomace, fired bricks.

C.A. 71

Use of Metakaolin and Fired Brick Waste in Geopolymer Production for Sustainable Construction

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Global interest to develop durable building materials with low CO_2 emissions makes geopolymer materials a friendly alternative to conventional construction materials. In this context, this study presents an experimental investigation into the properties of geopolymer binders prepared using metakaolin (MK) and red clay brick waste (RBW). A series of mixes with varying contents of RBW up to 100% as metakaolin replacement was prepared to assess several properties, such as, water absorption, compressive strength, thermal conductivity, and fire resistance. The experimental outputs signified that 30% RBW replacement exhibited good mechanical properties and superior thermal insulation compared to conventional cement, with lower thermal conductivity values and good fire resistance. Therefore, there is great potential for transforming red brick waste into a readily available aluminosilicate resource for use in geopolymer materials.

Keywords: Clay brick waste, Metakaolin, Geopolymer, Building materials.

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C.A. 72

Composition réfractaire à haute teneur en alumine pour matériaux monolithiques

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Ce travail est relatif à une composition réfractaire pour les matériaux monolithiques, notamment pour la préparation des bétons réfractaires caractérisés par des hautes teneurs en alumine. Ces bétons réfractaires sont destinés pour la protection des fours et des chambres de combustion, ils assurent la protection des installations et la protection physique du personnel de la matière chaude et l'extérieur de l'outil de traitement, les matériaux assurent aussi une isolation de manière à réduire les pertes calorifiques liés à l'utilisation de combustibles.

Les matériaux réfractaires monolithiques doivent posséder un certain nombre de propriétés complémentaires pour résister aux sollicitations qu'elles subissent en service. En général, le comportement des réfractaires est surtout gouverné par les phénomènes de corrosion par conséquent les caractéristiques essentielles mises en jeu sont leur composition chimique, minéralogique, leur microstructure et la morphologie de leur réseau poreux qu'ils développent au cours de leur mise en place.

Le domaine des matériaux réfractaires connait un développement intense des applications industrielles utilisant la technologie des monolithiques, il s'agit d'élaborer des revêtements à base de bétons incorporant dans leurs formules de base des liants hydrauliques ou chimiques. Cette technologie offre plusieurs avantages, le premier est la rapidité de l'exécution de la mise en œuvre et la facilité de la maçonnerie liée à l'utilisation des bétons réfractaires. Le second avantage est une économie d'énergie car il s'agit de matériaux non façonnés ne nécessitant pas de phase de mise en forme ni de traitement thermique préalable avant toute utilisation.

Ce travail est consacré à élaborer une nouvelle composition réfractaire caractérisée par l'utilisation d'une source de magnésium, cette source est apportée par les minéraux composant le talc ä savoir la chlorite et la dolomite, ces deux sources de magnésium jouent un rôle primordial, elle permettent de conférer à la matrice une microstructure unique donnant aux matériaux réfractaires des propriétés thermomécaniques excellentes et une usure uniforme. Ladite composition offre à des températures d'utilisation inférieure 1350°C une matrice ayant une microstructure exceptionnelle caractérisée par le développement de phases minérales très résistantes aux chocs thermiques il s'agit de la composition cordiérite-mullite, cette composition confère au béton constituant le revêtement réfractaire une résistance mécanique précoce et suffisante nécessaire pour la mise en œuvre démarrant ä partir de 1150°C (température d'utilisation pour certains procédés industriels), alors à haute température, la matrice est renforcée par le développement d'une phase minérale ayant une microstructure mullitique.

Keywords: Matériaux réfractaires, Bétons réfractaires, monolithiques

C.A. 73

Behavioral studies of Phosphate Sludge-Incorporated Geopolymer Concrete Submitted to Elevated Temperatures

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Geopolymer concretes have been increasingly used as a suitable alternative in industrial sector. However, if geopolymer concrete is mixed using a single feedstock, its performance is often severely limited by the physical/chemical characteristics of the feedstock. Thus, it is judicious to integrate feedstocks derived from industrial solid wastes to elaborate geopolymer concrete. In this study, untreated phosphate sludge (UPS) and Metakaolin (MK) were used to prepare sodium and/or potassium-activated unitary and binary geopolymer concretes and the microstructure, physical properties, and high-temperature performance were systematically investigated. The results showed that incorporating 50% of UPS significantly enhances the mechanical properties of geopolymer concretes with a 28-day compressive strength reaching 5.49 MPa. After treatment at 800°C, the elaborated concrete transformed from amorphous and semi-crystalline gel structures to a crystalline structure, regardless of the mix designs. Geopolymers activated with mixed alkali metals (Na/K) showed thermal shrinkage features, enabling structural compaction with minimal density loss, which is beneficial for their mechanical properties below 500°C. The abundant CaO in the UPS acts as a self-fluxing component to decrease the sintering temperature during geopolymer fritting, thus reducing temperatures that cause unexpected stiffness loss.

Keywords: Binary geopolymer concrete; Untreated phosphate sludge; High temperature; Mechanical properties

C.A. 74

Toxicology of Woods Extracts Characterisation by InfraRed Spectroscopy

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We show in this article, that it seems to be a link between certain spectral bands obtained with infra red spectra of wood dry extracts and their toxic effects on the skin, for asthma phenomenon appearance or ethmoïd bone cancer appearance. Extracts are coming from wood commonly used in Morocco. Article shows that the bands at 1415 cm^{-1} (organic acids) and 1771 cm^{-1} (organic anhydrides) are correlated to the three studied toxic effects, the band 1415 cm^{-1} (organic acids) is correlated with the onset of asthma or ethmoïd bone carcinoma appearance while the 1635 cm^{-1} (aliphatic benzene) band is linked only with the ethmoïd bone carcinoma appearance. These studies help to identify responsible bonds, presents in the molecules issue from woods extracts, and their toxic potential.

Keywords: wood toxicity**,** wood extracts toxicity, toxicity and IR spectra

C. A. 75

New method for Preparation of BiOCl-based film with exposed facets (110). Application in adsorption of the Azo dye (Azorubine) in water

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In this study, a new BiOCl-based film was prepared by simple precipitation method from a mixture of acrylamide, tragacanth gum, and Bismuth nitrate with varied concentrations. Characterization techniques such as X-ray diffraction (XRD), Fourier Transform Spectrometer (FTIR), and Scanning Electron Microscope (SEM) were used to study the effect of Bismuth nitrate concentration (0,3,5,7 and 10wt%) on prepared films' composition, microstructure, and 3D structure. The BiOCL-based film with a positively charged surface, three-dimensional structure with exposed facets (110), and porous microstructure was prepared with 3 Wt % of bismuth nitrate. The BiOCL film was tested for the adsorption of anionic azorubine dye in water. The result shows an adsorption activity of BiOCl film with a high removal rate of 99%. The influence of the dye concentration and temperature on the adsorption capacity was studied. The azorubine adsorption process is consistent with the Langmuir adsorption isotherm with the pseudo-second-order kinetic characteristics.

The high adsorption capacity of the prepared adsorbent towards azoribine is due to the porous microstructure and 3D structure of the BiOCl-based film favoring chemical interactions between the adsorbent and the anionic dye.

We can conclude that the film-BiOCl has the potential, to be used as an adsorbent for wastewater treatment and purification processes to eliminate emergent contaminants.

Keywords: BiOCl-film, Adsorption, Azorubine, Kinetic studies, Adsorption isotherms.

C.A. 76

Study of the hygroscopic character of fertilizer via impedance spectroscopy

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Fertilizers are chemical compounds intended to supplement plants with nutrients to improve their growth and increase crop yield and quality.

The combination of several elements (nitrogen, potash and phore) is more effective for plants than the action of each element used alone. These elements are found naturally in the form of phosphate, nitrates and various potassium salts.

Diammonium phosphate (DAP), monoammonium phosphate (MAP), triple super phosphate (TSP) and single super phosphate (SSP) fertilizers, derived from natural phosphate, are the most widely used products in soil enrichment of crops with essential nutrients, such as phosphorus (P). DAP and MAP also contain nitrogen (N), another essential plant nutrient.
Mono-ammonium phosphate (MAP) is a common source of phosphorus and nitrogen used. It is made from the two most prevalent constituents in the fertilizer industry and has the highest P content of all solid fertilizers.

In this work we propose an original study involving the impedance spectroscopy of the solid, to analyze the hygroscopic nature of the fertilizer, we studied the electrical and dielectric properties of the MAP fertilizer (rated MAP 1) and after 10 days of stays of this fertilizer at room temperature we repeated the same study (rated MAP2).

Indeed, the difference is clearly manifested in the electrical and dielectric behavior of the fertilizer after 10 days, via electrical modeling, ionic conductivity, permittivity and loss tangent.

Keywords: Fertilizers; impedance spectroscopy; electrical properties; monoammonium phosphate (MAP).

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C. A. 77

Electrical Properties Of MIS Structures On GaAs Passivated By A Silicon Nitride Deposited By The PECVD Technique At A Low Frequency And High Frequency

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The evolution of information and communication systems are directly linked to electronic and optoelectronic technologies, themselves based on semiconductor technologies. Among these semiconductors is the GaAs, which has a direct gap (1.42 eV), giving it excellent optical properties. Despite the potential of the material, many challenges remain and GaAs Technology faces significant challenges, in particular the chemical and electrical properties of the native oxide layer (~ 2 nm thick) on the surface GaAs (on all III-V surfaces) induces avery high density of surface states greater than 1012 $cm^{-2}.eV^{-1}$. These states prevent the use of III-V family semiconductor devices and decrease the performance of the component (MISFET). Several works have been carried out in order to understand the origin of the Fermi level anchoring, and to find a method for treating the surface of GaAs making it possible to reduce the density of the interface states to a level sufficient to improve the performance of devices sensitive to surface conditions, in addition to the fragility of these waffles. These factors limit profitability and increase the cost of integrated circuits.

It is in this perspective that our work takes place. Our main objective is to find a GaAs surface treatment process that will reduce the density of the interface states to a sufficient level. For this, we were interested in new passivation techniques of the GaAs surface, based on the use of silicon nitride deposited by PECVD low frequency and high frequency, that is to say that we have chemically passivated the surface GaAs with sulfur in the presence of oxygen, in order to ensure high stability and to have a protective insulating layer on the surface of our semiconductor. In order to characterize these structures, C-V measurements were carried out.

Keywords: Density in the interface Passivation, PECVD, MIS structure, Measure C-V.

C.A. 78

Synthesis, Characterization, and Investigation of Optical and Mechanical Properties of Biocomposite Films

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The growing use of particle/polymer composite films in recent years is driven by their distinctive properties resulting from the combination of the organic matrix. These films are highly versatile and can be used in a wide range of fields, including the environment, electrochemistry, protective clothing, optical devices and aerospace. In this study, biocomposite films were synthesized using polymers reinforced with microcrystalline cellulose (MCC) particles at different mass concentrations. The films were analyzed using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDS). The results showed that the films had partially dispersed and exfoliated structures. Increasing the MCC content led to a decrease in water solubility, absorption coefficient and transmission percentage, while the cut-off energy increased. Furthermore, the incorporation of MCC led to stiffer materials with increased tensile strength and Young's modulus. In conclusion, biocomposite films reinforced with MCC particles demonstrate enhanced properties, making them an attractive proposition for food packaging.

Keywords: Biocomposite films; optical properties; mechanical properties.

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C.A. 79

Rare effect on structure and dielectric proprieties in $RFeTiO_5$

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In the foreseeable future, dielectric materials are poised to offer heightened energy storage capabilities. Optimal choices for high-power energy storage applications entail dielectrics characterized by robust breakdown strength, minimal polarization hysteresis, and a moderate dielectric constant [1]. In pursuit of such advancements, we delved into the exploration of oxide compounds employing the solid-state synthesis method. These compounds, falling within the realm of oxides, exhibit exceptional magnetic and electrical properties, rendering them intriguing both from fundamental and technological standpoints. Their potential extends across various applications, encompassing multiferroic devices, spintronics, and high-energy-density cathode materials.

The crystal structure and dielectric properties of RFeTiO5 with (R= Pr, Nd, Gd). The crystal structure was refined using X-ray powder diffraction data and found to be in the orthorhombic Pbam space group with decrease in the cell parameters. The dielectric properties of the samples were studied at various temperatures and frequencies. The frequency dependence of the real and imaginary parts of the complex permittivity, impedance, modulus, and ac conductivity were investigated to determine the possible mechanism that describes the dielectric properties of RFeTiO5 and to probe the origin of the observed decrease. The study found that the microstructure consists of high-conductive grains and low-conductive grain boundaries, as well as the Maxwell–Wagner relaxation process. The hopping mechanism occurring in grains and grain boundaries was determined using the real part of the ac conductivity, and two temperature regions were distinguished.

Keywords: Solid state; Impedance; Dielectric spectroscopy; ac-conductivity; Compound;

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C.A. 80

Light absorption behavior and dielectric properties of $(Mg_{1-x}Ni_x)_4Al$ Layered double hydroxides $(0 \leq x \leq 1)$

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Lamellar double hydroxides (denoted LDH) are anionic clay-like compounds, Their corresponding chemical formula is: $[M_{1-x}^{2+}M_x^{3+}(OH)_2](A^{m-})_{\frac{x}{m}}.n\,H_2O$, where M^{2+} and M^{3+} are di and tri-valent metals respectively, M^{3+} ions produce an excess of positive charged layers which is neutralized by a compensating anion (A^{m-}) as CO_3^{2-}, SO_4^{2-}, Cl^- or NO_3^-. They are easy to synthesize, non-toxic and inexpensive, and among the materials likely to provide a solution in the treatment and recycling the effluents by using them as adsorbents or as catalysts.

In this study, Four phases of carbonate-intercalated Layered Double Hydroxides (LDH), based on magnesium and aluminum, with $\frac{M^{2+}}{M^{3+}} = 4$, have been successfully intercalated with nickel as a second divalent metal cation at different percentages (0%-50%-100%) by “coprécipitation” method at pH=10. The structural properties of the synthesized (Mg–Ni–Al–LDH) have been studied by using powder X-ray diffraction (XRD), Fourier transform infrared (FT-IR), respectively. In addition, the electrical/dielectric properties investigated are determined using impedance spectroscopy (IS) and the light absorption behavior are studied by diffuse reflectance spectroscopy.

This study has shown that the insertion of second bivalent metal into LDH matrices could increase their possible use in dielectric application and photo-catalysis.

C.A. 81

Elaboration and dielectric characterization of Aurivillius phase doped with rare earths

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As new needs arise in electrical engineering including pulsed power and directed energy, much researches concerning the development of new dielectric materials has been made in recent years, this materials are needed to reduce the size and cost of electrical assemblies, that is why the general theme of this researches is the obtention of low-cost reliable multilayer ceramic capacitors with a volume capacitance as high as possible.

$Sr_{(1-x)}Ln(x)Bi_2Nb_2O_9$ (Ln = rare earth) is a member of Aurivillius ferroelectric oxide family with space group P4bm at room temperature, that can be used as materials with high dielectric properties. In this work the effect of rare earth doped in the $Sr(1-x)Ln(x)Bi_2Nb_2O_9$ on the dielectric properties was investigated. Samples were prepared Using high temperature solid state reaction. Single-phase compound formation was confirmed by preliminary X-ray structural analysis. The surface morphology recorded by scanning electron microscope at room temperature exhibits a dense uniform grain distribution on the surface of the samples.

It has been observed that the incorporation of rare earth ions reduces the dielectric maxima. It further increases the degree of diffusiveness and lowers the temperature of dielectric maxima as a result of the introduction of additional random field via created point defects.

C.A. 82

Development and characterization of new oxide material: Electrical, magnetic and optical studies

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This study investigates the properties of Li_4ABO_6, focusing on its structure, dielectric behavior, and ionic conduction. The studied phase was synthesized via a solid-state route at high temperature, the compound exhibits a complex morphology with varying aggregate sizes. Ultraviolet-visible spectroscopy reveals electronic transitions attributed to A^{3+} ions, with a calculated gap band of approximately 2.01 eV. Dielectric analysis across a range of frequencies and temperatures highlights grain and grain boundary effects, with impedance spectroscopy confirming electrical inhomogeneity. The ionic conductivity of Li^+ ions is linked to bulk resistance, supported by Jonscher's law. Activation energy for conduction is determined as Ea = 0.57(1) eV, consistent with migration barrier energy values obtained from Bond Valence Path Analyzer (BVPA) analysis. These findings contribute to understanding the conduction mechanisms in Li_4ABO_6.

Keywords: Structure, X-ray diffraction, Dielectric, Li_4ABO_6.

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C.A. 83

Synthesis, Characterization and investigation of electric and dielectric properties of carbonate intercalated Mg-Al Layered Double Hydroxide with different molar ratios

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Anionic clays also called Lamellar Double Hydroxides (LDH) are among of materials that provide a solution in the treatment and recycling the effluents by using them as adsorbents or catalysts. Their corresponding chemical formula is: $[M^{2+}_{1-x}M^{3+}_{x}(OH)_2](A^{m-})_{\frac{x}{m}}.n\,H_2O$, M^{II} and M^{III} are divalent and trivalent metal ions, respectively, A^{n-} is the exchangeable hydrated anion located in the interlayer gallery for charge balance.

In this study, LDH materials based on Mg^{2+} and Al^{3+} was synthesized by the co-precipitation method at constant pH with Mg/Al =2, 3 and 4 molar ratio. Subsequently, they were characterized by X–ray diffraction, Fourier transform infrared spectroscopy and thermogravimetric analysis.

The electric and dielectric properties of the samples such as electrical conductivity, dielectric constant and dielectric loss tangent were investigated by impedance spectroscopy.

The study of the effect of the ratio showed a more conductive behavior in the direction R=4> R=3> R=2, over the entire measurement interval. As for the dielectric properties, the $Mg_4Al\text{-}CO_3$ phase has significant permittivity compared to the other phases over the entire frequency range with energy dissipation at 1 KHz.

Keywords: Mg-Al-LDH; impedance spectroscopy; dielectric properties; electric properties; coprecipitation method.

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C.A. 84

Structure, electrical, and dielectric properties of $Ba_{1-x}Y_xTi_{(1-x/4)}O_3$ ceramics sintering at low temperature

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The sintering temperature of $BaTiO_3$, prepared by solid-state reaction route, is in general above 1250 °C to achieve dense ceramic. In this regard, we investigate the effect of low sintering temperature on the electrical and dielectric properties of lead-free of $Ba_{1-x}Y_xTi_{(1-x/4)}O_3$ ($x = 0$ and 0.02) ceramics. Tetragonality of these structures was determined through powder X-ray diffraction and Raman analysis. $BaTiO_3$ has a uniform grain size, but the doped sample consists of a different shape and size with homogeneous morphology and dense microstructure, as observed by scanning electron microscopy. Through dielectric measurements, the Y-doped BT ceramic has a higher Curie temperature (T_C) and dielectric constant (124 °C and 7000) at 1 MHz, which explains a dense microstructure. Besides, the dielectric loss was less than 2.10^{-2} in the entire temperature range from room temperature to 300 °C.

Keywords: Perovskite; Structural; Y-doping ;Dielectric properties

C.A. 85

Structural, Vibrational, and Magnetic Characterization of Double Perovskites La_2NiMnO_6 and La_2CoMnO_6

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Double perovskite oxides with various ions located in the A or B sub-lattices have garnered significant interest due to the many fascinating discoveries stemming from them, such as multiferroic behavior, colossal magnetoresistance effect, ferroelectric/piezoelectric effect, and oxygen ion transport and storage properties for solid oxide fuel cells and water splitting catalysis. In particular, La_2NiMnO_6 (LNMO) and La_2CoMnO_6 (LCMO) have been intensively studied because of their unique magnetic, electric, magnetoelectric, magnetoresistance, and multiferroic properties. In this study, the effects of chemical composition on the structural, vibrational, and electronic properties of the manganese powder La_2CoMnO_6 based on 3d double perovskite, prepared by high-temperature solid-state chemistry, are examined. The crystalline structures of La_2CoMnO_6 were determined by X-ray diffraction (XRD) and are refined into a monoclinic structure of the P21/n space group. In this model, the cobalt and manganese (Mn^{4+}) atoms are placed at the Wyckoff 2b (0, 0, 1/2) and 2a (0, 0, 0) positions, respectively, while the lanthanum (La^{3+}) and oxygen (O^{2-}) atoms occupy different 4e (x, y, z) positions. The dynamic and structural properties of the studied compounds were analyzed by infrared spectroscopy, Raman, and XRD. The infrared spectra reveal characteristic peaks corresponding to the stretching modes of the Mn-O and Co/Ni octahedra. The XRD analyses confirmed the crystalline phase and symmetry of the studied materials.

Keywords: Double perovskites; Magnetic properties; High-temperature solid-state chemistry; Structural properties; Vibrational properties.

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C. A. 86

The electronic, structure, magnetic and optical properties of TiO_2 anatase : DFT study

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In this work, the electronic structure, magnetic and optical properties of the anatase phase of titanium dioxide (TiO_2) were etudiée by the Density Functional Theory (DFT) method, using the GGA+U method. As a result, the magnetic electronic properties show that anatase is a non-magnetic semiconductor with an indirect gap of 3.202. Optical properties such as dielectric function, refractive index, extinction coefficient, reflectivity, absorption coefficient and conductivity were found to be 8.21, 2.91, 1.98, 0.532, 517000 cm^{-1} and 8.9 fs^{-1} respectively. These results are in agreement with the available experimental results.

Keywords: Titanium dioxide (TiO_2); DFT; electronic properties; structure properties magnetic properties; optical properties

C. A. 87

Chemical durability and optical properties of MnO-Sb_2O_3-B_2O_3 glasses

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Heavy metal oxide glasses based on antimony have attracted a great deal of interest in recent years because of their low phonon energy, high refractive index and broad optical transmission spectrum.

Glasses with high antimony content combined with glasses such as borate or phosphate glasses, are of significant technological interest. They have been recently considered as potential materials for non-linear optical applications, such as power limiters and ultrafast optical switches, due to their high non-linear optical susceptibility

We have developed new glassy materials based on antimony and boron oxide by elaborating and analyzing the MnO-Sb_2O_3-B_2O_3 ternary system.

Glasses composed of xMnO-(40-x)Sb_2O_3-60B_2O_3 and xMnO-50Sb_2O_3-(50-x)B_2O_3, where $5 \leq x \leq 10$ mol%, were produced using a melt-quenching technique. X-ray diffraction analysis was used to confirm the amorphous nature of the glasses.

This work focuses on the chemical durability in various leaching solutions and on the study of the optical properties of the prepared glasses.

Keywords: Glass, Borate oxide, Antimony, XRD, Chemical durability, Optical property

C. A. 88

Vibrational spectra, Optical and Magnetic Properties of the Vanadium (IV) Oxyphosphates (α, β) - $M(VO)_2(PO_4)_2$ (M = Co, Ni)

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Vanadium oxyphosphates have attracted worldwide attention in recent years due to their wide range of applications. These oxyphosphates are promising materials for applications in catalysis [1], Li-ion batteries [2], Na-ion batteries [3] and corrosions [4].

We reported in a previous work the syntheses and crystal structures of vanadium (IV) oxyphosphates $M(VO)_2(PO_4)_2$ (M = Co, Ni) [5]. For each compound, two phases, named α and β, have been stabilized at room temperature, then characterized. Their crystal structures were refined, in monoclinic $P2_1/c$ space group, using powder X-ray diffraction data. All these structures consist of a three-dimensional (3D) framework built up of infinite chains of tilted corner-sharing $[VO_6]$ octahedra, cross-linked by corner-sharing $[PO_4]$ tetrahedra. The M^{2+} ion (Co^{2+}, Ni^{2+}) is located in a triangular based antiprism which shares faces with two $[VO_6]$ octahedra. Vibrational study of these oxyphosphates is in good agreement with structural results and confirms the existence of the infinite -O-V-O-V-O- chains. Their optical absorption study confirmed the presence of V^{4+}, Co^{2+} and Ni^{2+} ions in octahedral environments. The optical band gap energy is estimated using the Tauc method. The magnetic study revealed an antiferromagnetic behavior at low temperature with T_N = 32K for Co-compound and T_N = 9K for Ni-compound.

Keywords: Vanadium oxyphosphates, Raman-Infrared, Optical Properties, Magnetic Properties.

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C.A. 89

Square planar coordination of cobalt (II): Synthesis, structural characterization, optical and magnetic properties of novel phosphate $Ba_2CoFe_2(PO_4)_4$

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Phosphates have captured considerable attention owing to their diverse applications in catalysis, energy storage, and electronics. In this study, a novel compound containing barium, cobalt, iron, and phosphate components was successfully synthesized in single-crystal and polycrystalline forms. Single-crystal X-ray analysis revealed that the compound adopts a monoclinic crystal structure with the $P2_1/c$ space group. This structure is intricately composed of interconnected FeO_6 octahedra, CoO_4 square planar units, CoO_5 square pyramidal units, and PO_4 tetrahedra, forming a three-dimensional lattice with tunnels along the a-axis for Ba^{2+} cations.

The polycrystalline variant, prepared using the sol-gel method, displayed a distinct X-ray diffraction pattern, refined via Le Bail method. Scanning electron microscopy was employed to explore its morphology and elemental distribution. Additionally, Infrared and Raman spectroscopies provided insights into chemical bonding. The magnetic behavior was antiferromagnetic below $T_N \sim 20$ K. Optical measurements revealed a direct bandgap with an energy E_g of 2.83 eV.

C. A. 90

Study and Characterization of Iron Orthophosphate for Energy Storage Applications

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The chemistry of orthophosphates $A^{II}M^{IV}(PO_4)_2$ (A^{II} =Ca, Sr, Pb, Ba; M^{IV} = Ge, Ti, Mo, Sn, Hf, Zr) [1-5] phosphates have been intensively studied during the past two decades for applications including catalysts, ion conductors, optical. Note that phases with a mixing of Sb^{V} and M'^{III} ions in the octahedral M sites of the $A^{II}M^{IV}(PO_4)_2$ yavapaiite structure types were studied here for the first time. Recently, the structural characteristics by X ray powder diffraction (XRD) study using the Rietveld method for three newly synthesised $A^{II}(Sb^{V}_{0.5}Ga^{III}_{0.5})(PO_4)_2$ (A= Ba, Pb and Sr) [6] phases were realised . All materials exhibit the yavapaiite type structure. In a continuation of our search concerning phosphates with interesting physical applications, the principal objective of the present study was the structural determination, using Rietveld refinement of the (XRD) patterns, of the $BaSb^{V}_{0.5}Fe^{III}_{0.5}(PO_4)_2$. The phase crystallize in the monoclinic C*2/m* space group (Z = 2; a = 8.1661(1) Å; b = 5.1934(3) Å, c = 7.8212(3) Å; β = 94.51(1)°, V = 331(1) Å^3). Its crystal structure consists of layers, running along the (ab) plane, built up of corner-connected $Sb(Fe)O_6$ octahedra and PO_4^{3-} tetrahedra, the Ba atom is coordinated to ten oxygen atoms with Ba-O distances ranging from 2.76 Å to 3.11 Å. The Infrared and Raman spectroscopy analysis were performed based on theoretical group analysis considering the C_s site symmetry. The assignment and discussion of the observed frequencies were done by comparison to other materials of the yavapaiite family. The UV-visible properties showed direct and indirect optical gap energies of values, 3.25 to 2.96 eV.

Keywords Crystal structure; IR-Raman spectroscopy; Phosphate; Rietveld refinement; UV–Visible.

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C. A. 91

Lithium decorated 2D orthorhombic (o)-B2X2 monolayers for hydrogen storage: first principles calculations

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Over the last few years, scientists and researchers have shown significant interest in the search for suitable two-dimensional (2D) materials that can store hydrogen efficiently, possess high gravimetric capacity, and demonstrate excellent physisorption properties for hydrogen molecules. In this regard, we have investigated, using density functional theory calculations (DFT), lithium decorated 2D or- thorhombic (o)-B2X2 monolayers (X≡P or N atoms) as possible solid-state and lightweight candidate materials for hydrogen storage. Our findings reveal that the o-B2P2 exhibits semi-metallic behavior, while the o-B2 N2 has a semi-conductor state with a band gap of 0.64 eV. During the lithium decora- tion process, lithium adatom exhibited a strong binding energies of -3.09 and -1.98 eV for o-B2P2 and o-B2N2 , respectively. These energies are significantly higher than the cohesive energy of Li (-1.63 eV), suggesting the absence of lithium-clustering formation. Furthermore, the lithium decoration process effectively enhances the adsorption of H2 molecules on both materials (e.g., 32H2@B2P2 and 24H2@B2N2), leading to a high gravimetric hydrogen storage capacities of 8.18 and 9.7 wt%, respectively. With reference to the average hydrogen adsorption energy of 0.18 (for 32H2@B2P2) and 0.20 eV (24H2@B2N2), the corresponding desorption temperatures were found to be 126 and 148 K. Based on these results, it can be deduced that Li-decorated (o)-B2P2 and (o)-B2N2 hold great promise as highly effective substrates for H2 storage.

Keywords: Hydrogen storage, 2D Materials, Energy storage, Decoration strategies.

C. A. 92

Advanced Cathode Materials for Next-Generation Batteries

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Cobalt plays a vital role in conventional cathode materials, by stabilizing the crystal structure of cathode materials and preventing Li/Ni intermixing, etc... However, the cobalt content of cathode materials in lithium-ion batteries must be reduced or eliminated due to the scarcity of cobalt resources, high price fluctuations, and other factors like its toxicity and some environmental and ethical concerns [1,2]. So, to generate superior cathode materials for lithium-ion batteries at a lower cost and higher energy density, researchers have identified nickel-rich and cobalt-free cathode materials as their primary target.

In this work, our objective primarily focuses on how removing cobalt affects the material properties of Ni-rich cathode materials. For this reason, we designed $LiNi_{0.8}Mn_{0.15}Al_{0.05}O_2$ (NMA), a cobalt-free and nickel-rich cathode material that was successfully synthesized using sol-gel and co-precipitation methods. The crystalline phases are characterized by different techniques. The synthesis methods demonstrate that the NMA performed by the co-precipitation method provides promising properties in terms of crystallinity and cation mixing degree.

Keywords: Cobalt-Free, Nickel Rich, Cathode Materials, Lithium ion-batteries.

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C. A. 93

Synthesis and Design of Novel Solid Electrolytes for All-Solid-State Li Batteries

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All-solid-state batteries have garnered significant attention as promising energy storage devices due to their potential for enhanced safety, increased energy density, and extended cycle life compared to traditional lithium-ion batteries. Among the various components crucial for the functionality of All-solid-state batteries, solid electrolytes play a critical role in enabling efficient ion transport while ensuring mechanical stability [1]. Lithium-conducting NASICON-type materials have emerged as promising candidates for solid electrolytes in All-solid-state batteries due to their high ionic conductivity, wide electrochemical stability and compatibility with diverse electrode materials [1].

In this study, novel LiZr2(PO4)3 solid electrolytes were synthesized by employing solid-state reaction and sol-gel methods, incorporating dopants from the fourth row of the periodic table. The primary objective was to assess the influence of doping and synthesis techniques on ionic conductivity. Characterization of the crystalline phases using various analytical techniques revealed that solid-state reaction coupled with Gallium and Calcium doping yielded the most promising results, showing notable improvements in the ionic conductivity.

Keywords: LZP Nasicon, inorganic solid electrolyte, All-Solid-State Lithium batteries.

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C. A. 94

Powdered Milk Production Using Coupled Cryo-Concentration and Freeze-Drying Processes

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In the food industry, many raw materials are submitted to one or more drying processes. Several dehydration methods are now available, offering advantages such as speed and long-term preservation of raw material quality. Freeze-drying offers particular advantages in terms of quality and shelf-life by removing water at low temperature under vacuum. However, this technique has limitations from a scientific and technological point of view, due to its high cost, as well as the extended duration of cycles [1]. To improve the efficiency of product dehydration, it is common practice to couple freeze-drying with other concentration methods, widely used as a preparation step prior to drying. This approach makes it possible to further reduce the water content of products while minimizing the associated drawbacks. Various concentration processes are currently available, such as vacuum evaporation, reverse osmosis and, to a lesser extent, cryo-concentration, but each process has its own drawbacks.

The aim of this project is to develop a coupled cryo-concentration and freeze-drying process to produce milk powder. The advantage of coupling is to accelerate the freeze-drying cycle, by drying pre-concentrated solutions. Firstly, a process parameter study was carried out to evaluate the feasibility of separation and achieving maximum concentration by comparing block and progressive cryo-concentration results. Densimetry was used to measure solute concentration in the solution after separation. Secondly, a parametric study of the freeze-drying process was carried out at laboratory and pilot scale, to examine how the different parameters affect the dry matter content of the final product. This study was completed by correlating the results of the NIR/Karl Fisher methods. Experimental temperature data (T_f, T_g, $T_{,c}$) obtained in our previous work were used to optimize our processes [2]. Understanding and controlling these parameters enabled us to assess the impact of composition and define the limits of the study in terms of temperature and concentration. The resulting powders were then observed using a scanning electron microscopy (SEM). Finally, the optimization of freeze-drying cycles and the use of progressive cryo-concentration enabled us to improve the combined cryo-concentration/lyophilization process and significantly reduce freeze-drying time and cost.

Keywords: Powdered milk, Cryo-concentration, Freeze-drying.

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C.A. 95

Advancements in Wind Turbine Blade Design: A Critical Review of Structural Performance with plant-based fibers Hybrid Composites

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The global commitment to reducing gas emissions and transitioning to a more environmentally friendly industry has greatly intensified demand for wind energy[1–3]. Given this global imperative, the use of natural fibers in wind turbine blade design has received particular attention[4,5]. This comprehensive study aims to provide an overview of the current state of wind turbine blades, focusing on the significant results achieved in their design through the integration of natural fibers. As an example, the hemp fibers were explored in this study as a potential Moroccan biomass to develop composites reinforcement for blades. To do so, a structural analysis was performed with various draping scenarios. The optimal one showed a 20% reduction in weight between the old and new model, and a cost reduction of approximately 30% [4].

Finally, this study provides insights of the potential of other promising and available natural fibers that possess important mechanical characteristics and future opportunities and perspectives for innovation and optimization toward sustainable blade design.

Keywords: Natural fibers; Hybrid composite, FEA; Wind turbine blade.

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C.A. 96

Study of thermo-physical properties and cycling stability of D-Mannitol and D-sorbitol as PCMs

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Sugar alcohols (SA) are emerging as one of better energy storage materials for thermal energy storage (TES) application due to its phase change temperature ranges (15 to 245°C) and considerable phase change enthalpies of 100–430 kJ/kg. However, the main challenges include the low thermal response of the phase change materials (PCM) owing to its very low thermal conductivity values. In this paper, D-mannitol and D-sorbitol were a candidate material to be tested as PCMs. They are materials which has different morphological phases (polymorphism). In this work, β-form and δ-form were studied. Different polymorphic forms produce changes on melting point of D-mannitol and D-sorbitol. The identification and characterization of the starting products was analyzed using X-ray diffraction and the IR spectroscopy. The phase change temperature, enthalpy of fusion and the thermal stability under ambient atmospheres of the studied forms were determined using a coupled Differential Thermal Analysis (DTA) and thermogravimetric analysis (TGA). To test the reversibility of the process, a study of the recrystallization of different phases of these polyols was carried out in different binary solvent mixtures, using Differential Scanning Calorimetry (DSC).

Keywords: Polyols, MCP, latent heat, crystallization, thermal energy, energy storage

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C.A. 97

Synthesis Strategies and Electrochemical Performance of Mg_2MnO_4 for Zinc Ion Batteries: Unveiling Sustainable Pathways for Next-Generation Energy Storage

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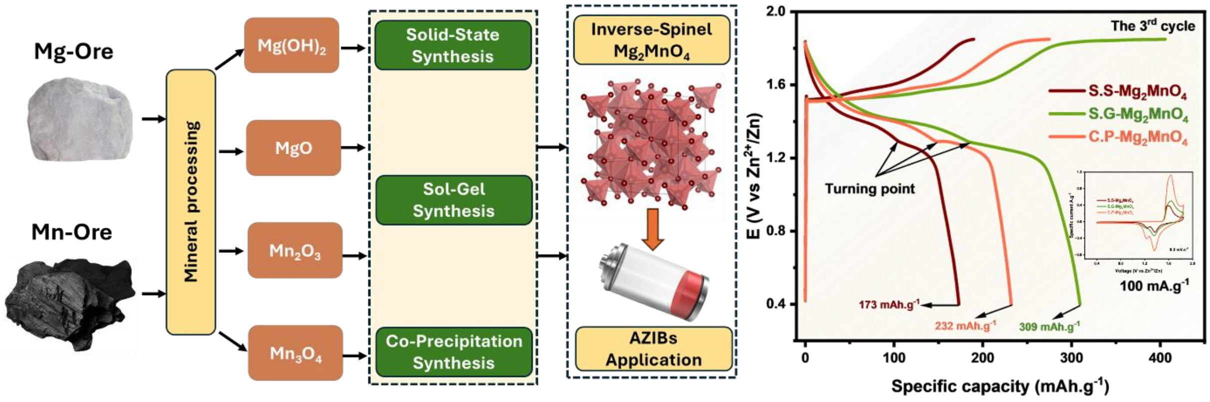
Manganese-based materials have emerged as promising cathode candidates for advanced zinc-ion batteries (AZIBs) due to their diverse crystal structures, various valence states, and high-voltage platforms. Among these materials, Mg_2MnO_4, rich in high-valence-state Mn^{4+}, shows remarkable discharge capacity and structural stability. However, the limited application of inverse spinel materials in AZIBs hinders their development. Here, we present a novel approach to synthesizing and comparing Mg_2MnO_4 with an inverse spinel structure. Three synthesis methods: solid-state (S.S-Mg_2MnO_4), sol-gel (S.G-Mg_2MnO_4), and co-precipitation (C.P-Mg_2MnO_4) were employed using natural sources. Magnesium and manganese were extracted and converted from crude ores to $Mg(OH)_2$, MgO, Mn_3O_4, and Mn_2O_3 through acid leaching and thermal decomposition process. As results, C.P-Mg_2MnO_4 exhibited a high discharge capacity of 708.93 mAh g^{-1} and capacity retention of 92% after 50 cycles at 100 mA g^{-1}. In contrast, S.S-Mg_2MnO_4 showed lower capacities of 353.64 mAh g^{-1} and S.G-Mg_2MnO_4 displayed instability during cycling under the same conditions. This study demonstrates a new pathway for synthesizing battery materials from natural resources, offering a promising avenue for designing high-performance AZIBs for durable applications.



Keywords: Magnesium ore; Manganese ore; leaching process; solid-state, sol-gel , co-precipitation, Inverse spinel, Mg_2MnO_4

C.A. 98

Diatomite based-binary salt hydrate for thermochemical energy storage

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The energy crisis poses many problems nowadays. The development of new materials to store energy became the main solution. Salt hydrate present a great option as materials to store energy especially salt-based chlorides. However, the energy storage density, cycling stability, cost and corrosive behaviour of chloride-based hydrated salts are the main technical challenges facing the application of these materials for thermal energy storage (TES) [1]. However, the impregnation of these salts into porous absorbent materials represents a key tool for solving these defects [2]. This paper seeks to develop low-cost thermochemical composites (CTCMs) based on natural diatomite and binary inorganic hydrated salts for TES application. Natural diatomite was used as support to stabilize the binary hydrated salts $CaCl_2 \cdot 6H_2O$ and $BaCl_2 \cdot 2H_2O$. Synthesis and microstructural characterization of binary@DT were presented. The composite TCM exhibited a great storage density.

Keywords: Thermal energy storage, Thermochemical energy storage, Diatomite, Binary hydrated salt.

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C.A. 99

Kinetic study of the elimination of Methylene Blue in aqueous solution by biosorption on Nicotiana Glauca.

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In this study, the easy and rapid adsorption of Methylene Blue (BM) dye from aqueous solution was investigated using Nicotiana glauca (NG) plant powder as a bio-adsorbent. This powder was characterized using various analytical techniques, such as X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), Fourier transform infrared spectroscopy (FTIR), and zero charge point determination (pHzcp). These analyses have enabled us to gain a better understanding of the structure and physicochemical properties of this natural adsorbent.

Optimum values for the most important experimental parameters (pH of the initial solution, quantity of adsorbent and contact time) were established for each batch of samples at room temperature (20°C ± 2°C). The kinetics of the adsorption process follows the pseudo- second-order kinetic model, and the Langmuir isotherm model is best suited to the adsorption of BM dye on NG plant powder. The maximum adsorption capacity, calculated in this case, is close to 100 mg/g. This value is very interesting compared with other results recorded for other adsorption media in the same range.

In addition, the adsorption process was spontaneous, thermodynamically favorable and endothermic. These results demonstrate the potential of NG biomass as an effective adsorbent for the treatment of methylene blue-contaminated effluents.

Keywords: Methylene blue; Nicotiana glauca; adsorption and Langmuir model.

C.A. 100

Developing and examining arginine-doped polyaniline/SiO_2 for the adsorption of Orange G dye from aqueous solutions

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The objective of this study was to synthesize and characterize arginine-doped polyaniline/silicon dioxide (Arg-PANI@SiO_2). The composite was created by polymerizing aniline monomer with SiO2 particles in the presence of arginine, utilizing sodium persulfate as an oxidizing agent. Various analytical techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller (BET), and PZC were employed to elucidate the properties of the developed composite material. Furthermore, the Arg-PANI@SiO_2 composite was applied to remove OG (reactive orange G) from aqueous solutions. The adsorption of OG onto Arg-PANI@SiO_2 was found to be influenced by factors such as the dosage of the adsorbent, pH levels, contact duration, pollutant concentration, and temperature. Experimental data exhibited excellent agreement with pseudo-second-order kinetics and the Freundlich isotherm. The maximum monolayer coverage capacity for OG onto Arg-PANI@SiO_2 was determined to be 387.16 mg/g. The adsorption of OG onto the composite occurred spontaneously through an endothermic process. The findings from this study strongly suggest that the synthesized Arg-PANI@SiO_2 hybrid composite has promising potential as an efficient filtration material for the effective removal of OG textile dye from aqueous solutions.

Keywords: Adsorption, Orange G dye, polyaniline.

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C.A. 101

Innovative valorization of EPS waste for oil/water separation using electrospinning and [Im, Br] ionic liquid

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The aim of this study is to develop an innovative membrane for separating oil-water mixtures, based on Expanded polystyrene (EPS) waste collected from food and electronic packaging and functionalised by the ionic liquid 3-hexyl-1-methyl-1H-imidazol-3-ium Bromide [Im,Br] . Different percentages of IL were added (1%, 3%, 6%, 12%). The surface chemistry, surface morphology, wettability and emulsion separation performance of the developed membranes were investigated in detail. The fiber diameter decreased considerably after the addition of the ionic (passing from 1,09 µm to 0,442µm). Surface properties showed a transition from hydrophobic to super-hydrophobic properties, as demonstrated by water contact angles ranging from 116° to 154° degrees. These results demonstrate the successful functionalization of recycled EPS-based membranes by the addition of ionic liquid, leading to surfaces that are highly capable of repelling water. This research contributes to the advancement of sustainable solutions for oil-water separation during oil spill incidents, as well as recovering EPS waste.

Keywords: Calcium EPS waste, Recycling, offshore, separation, Electrospinning, ionic liquid

C.A. 102

Novel Argan spinosa Leaves Modified with Citric Acid for Highly Efficient Removal of Crystal Violet Dye from Wastewater

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Over the recent decades, water contamination has surged, emerging as a critical global concern. This study focuses on the removal of crystal violet (CV) dye from water, employing citric acid-modified argan spinosa leaves (CA@Arg-Sp) as effective adsorbents. The morphology and surface chemistry of the newly functionalized argan leaves denoted as CA@Arg-Sp, were scrutinized using SEM, FTIR, and TGA/DTA. Additionally, thermal stability assessments revealed that the CA@Arg-Sp material remains structurally intact up to 260 °C. The study investigated the efficiency of CA@Arg-Sp in eliminating CV dye from wastewater. Optimal removal, reaching 99.5%, was achieved at pH 7. Electrostatic attractions and hydrogen bonding were identified as crucial factors enhancing CV adsorption. Adsorption performance was further analyzed concerning adsorbent dosage, initial dye concentration, temperature, contact time, and pH. The Freundlich isotherm and pseudo-second-order models exhibited excellent fits in both isotherm and kinetic adsorption modeling. CA@Arg-Sp displayed a maximum adsorption capacity of 335.09 mg/g. Thermodynamic analyses affirmed the endothermic and spontaneous nature of the CV elimination process. Overall, the experimental findings support the conclusion that CA@Arg-Sp serves as a cost-effective, easily renewable, regenerable, and environmentally benign adsorbent for textile effluent purification.

Keywords: Citric Acid; Argan Spinosa Leaves; Functionalization; Adsorption; Dye.

C.A. 103

Application of response surface methodology for optimization of concentration process and removal of organic and mineral matter from olive oil mill wastewater by cryoconcentration

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The olive oil extraction generates two by-products, which are the olive pomace and olive vegetation water called olive oil mill wastewater (OMW). Due to their high organic loads, and high amounts of organic acids and phenolic compounds, OMW are toxic for ecosystem and are considered one of the most harmful effluents produced by the food industry. The objective of this study is to develop a process for the treatment and valorization of OMW through cryoconcentration. This type of wastewater is characterized by high concentrations of organic and mineral substances. The treatment tests are carried out in four stages: cooling, freezing, sweating, and fractional melting. These steps allow for a thorough purification of the ice block produced by partially melting of the impure zones of concentrated solution pockets. In this study, a response surface methodology was used to optimize the parameters of three factors: Dry matter concentration (DM), cooling temperature (T_c), and the number of liquid solutions recovered during partial melting (N_{LF}). Sixteen different tests were carried out to evaluate the influence of each factor and the effect of their interactions on the recovery of organic matter (MO) and mineral matter (MM) in the initial liquid fraction ($F_{i=1}$), as well as their removal in the last fraction ($F_{j=3,4 \text{ and } 5}$). Three response models were successfully developed, two quadratic and one cubic, and their validity was confirmed by an analysis of variance (ANOVA). It is noted that all the models exhibit high values of coefficient of determination (R^2), ranging from 94.91% to 99.07% for the two quadratic models, and an R^2 of 98.13% for the cubic model. The results showed that the concentration value in the first recovered solution increased from 8.49% to 22.46% for the organic matter and from 2.20% to 4.71% for the mineral matter. In the last recovered solution, the dry matter concentration decreased from 10.51% to 0.18%. In conclusion, cryoconcentration can be successfully employed to help reduce the discharge of olive mill wastewater to zero while producing purified water for various purposes and valorizing the cryoconcentrated solutions obtained with high polyphenol concentration.

Keywords: Olive Mill Wastewater treatment; Cryoconcentration; Sweating; Organic matter; Mineral matter; Response Surface Methodology.

C. A. 104

Turning waste into wealth “Novel approaches for the use of goat dung in biostimulation and bioremediation”

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Controlling environmental pollutants, particularly heavy metals, is a significant worldwide issue. Bioremediation involves using plants to decrease pollutants and is seen as an environmentally friendly and economical approach. Goat excrement is gaining attention as a natural stimulant for bioremediation processes. It is a beneficial material rich in organic matter and nutrients that can enhance plant growth and aid in remediation processes. The objective of this review is to examine the wide-ranging uses of goat dung in bioremediation initiatives worldwide. This study explores the use of goat dung for absorbing and sequestering pollutants, and also its use as a biostimulant enhancing nutrient and plant growth, aiming to determine its environmental and economic benefits in bioremediation approaches.

By utilizing data from recent research, this review establishes that supplementing soil with goat manure can enhance crop productivity, and soil fertility, thus providing sustainable solutions to agricultural challenges. Furthermore, the evaluation explores the application of goat manure in bioremediation processes, with a specific focus on its potential to mitigate soil contamination and restore ecological balance. Through case studies and experimental trials, we establish the effectiveness of goat manure amendments in promoting the sequestration, absorption, and detoxification of various pollutants such as heavy metals, motor oils, and other polluant compounds.

Furthermore, this analysis is conducted on the environmental and economic benefits that are linked to the adoption of biostimulation and bioremediation techniques that incorporate goat manure. These encompass factors such as cost-effectiveness, minimal ecological footprint, and potential for expansion.

C. A. 105

Metal Recovery from Industrial Wastewater using Calcium Oxide and Cactus Combination

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In this study, we explore the synergistic potential of combining calcium oxide (CaO) and cactus for sustainable metal recovery from industrial effluents. Through a detailed examination of the unique properties of both calcium oxide and cactus, including their metal-binding capabilities and environmentally friendly attributes, we investigate the mechanisms underlying their cooperative action in metal removal processes. Drawing upon recent research and experimental findings, we assess the efficacy of the calcium oxide and cactus combination in extracting metals such as Al, Fe and Cd from wastewater streams. Furthermore, we analyze the optimization strategies and operational parameters for enhancing the efficiency of metal recovery using this novel approach. Additionally, we discuss the economic viability and environmental benefits of implementing calcium oxide and cactus synergy in industrial wastewater treatment systems. This study provides valuable insights into the development of sustainable and cost-effective methods for mitigating metal pollution in industrial wastewater, contributing to both environmental conservation and resource recovery efforts.

C. A. 106

Use of geraniaceae extract as a green inhibitor of steel corrosion in an acid environment

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Corrosion inhibition is one of the best techniques for protecting metals when they come into contact with aggressive media such as acids. The main drawback is toxicity. For this reason, the use of aromatic plant extracts as green inhibitors is being widely studied as an alternative.

The aim of our study was to evaluate the inhibiting power of geraniaceae extract against steel corrosion in an acid environment. After extraction, we sought to determine the chemical composition of the extracts using GC-MS and FTIR techniques. In order to determine the inhibitory power of our extract, we used electrochemical impedance spectroscopy and Tafel polarization methods (Figure) with a concentration range (50ppm - 200ppm) and a temperature ranging from 298 K to 328 K. A significant inhibitory effect was confirmed using these methods. The inhibitory efficacy of our extract increased with increasing concentrations, up to 96%.

C. A. 107

Arginine-polyaniline embedded jujube shells composite for outstanding Cr(VI) detoxification from wastewater

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A hybrid composite, denoted as Arginine-doped polyaniline@JS (Arg-PANI@JS), was created by performing an interfacial polymerization reaction using aniline on the surface of JS particles in the presence of arginine. This composite was subsequently characterized using energy dispersive X-ray spectroscopy (EDS), field emission scanning electron microscopy (FE-SEM), and Fourier transform infrared (FT-IR) spectroscopy. In the next step, the Arg- PANI@JS composite was used in Cr(VI) adsorption experiments, involving artificially contaminated solutions. The kinetics and equilibrium results were successfully described by a pseudo-second-order model and the Freundlich isotherm. An experimental batch adsorption setup was utilized to assess the effectiveness of the newly synthesized adsorbent in removing Cr(VI) ions from aqueous solutions. Under the conditions optimized for the experiment, employing 0.375 g·L-1 of Arg-PANI@JS and a Cr(VI) concentration of 20 mg·L-1 at pH 2 and 298 K. Furthermore, our assessment demonstrated that the Arg-PANI@JS composite can be readily regenerated using a NaOH solution and effectively reused for removing Cr(VI) from aqueous solutions. Consequently, these findings underscore the promising practical utility of the PANI@JS composite in wastewater treatment.

Keywords: Adsorption; Cr(VI) ions; polyaniline; JS; kinetic; Regeneration.

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C.A. 108

Efficient Adsorption of the Pharmaceutical Agent Diclofenac Sodium fromAqueous Solutions Using Layered Double Hydroxide as Promising SorbentMaterial

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Pharmaceutical products, notably anti-inflammatories, present a significant environmental concern due to their non-biodegradable nature as organic substances. After their therapeutic use, these pharmaceuticals can exert detrimental effects on the environment. The improper disposal of pharmaceuticals, whether through human excretion or inadequate waste management, contributes to the contamination of soil and water resources. Consequently, there is an urgent need for effective strategies to eliminate these pollutants from the environment to safeguard ecological balance and mitigate potential adverse effects on both terrestrial and aquatic ecosystems.

Thanks to its relevant properties, the application of layered double hydroxide (LDH) in the field of the environment has become a major concern for several laboratories, aiming to minimize the discharge of toxic substances. In this context, we focused on the removal of Diclofenac sodium (DS) through adsorption on a LDH of the ZnAl type.

The influence of various parameters such as contact time, initial DS concentration, adsorbent material mass, and solution pH on the adsorption process of the diclofenac sodium was investigated.

Keywords: Diclofenac sodium, Layered double hydroxide, Adsorption

C.A. 109

Sustainable corrosion protection: exploring an organic inhibitor for mild steel

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This research focuses on the development and characterization of an organic corrosion inhibitor specifically designed to offer robust protection to mild steel in hydrochloric acid environments. The study details a streamlined and efficient synthesis method and provides an in-depth examination of the chemical structure of the organic compound using techniques such as X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy and nuclear magnetic resonance (NMR) spectroscopy. To assess the effectiveness of this organic compound in inhibiting corrosion, experiments were carried out at varying concentrations in a 1M hydrochloric acid solution for mild steel, using potentiodynamic polarization and electrochemical measurements. The results indicated a proportional increase in inhibition efficiency with inhibitor concentration, correlating with a reduction in corrosion current density. Notably, the inhibitor showed maximum effectiveness at a concentration of 400 ppm, reaching an inhibition efficiency of 95.77%. The impact of temperature on inhibition efficiency was discussed over a temperature range from 298 to 328 K. Polarization measurements revealed that the synthesized inhibitor functions as a mixed-type inhibitor. This study combines an efficient synthesis process, comprehensive characterization and performance evaluations, highlighting the potential of this organic inhibitor to effectively protect mild steel against corrosion in aggressive environments [1].

Keywords: Hybrid materials, Corrosion inhibition, Mild steel, electrochemical study

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C.A. 110

Efficiency of nanocelluloses isolation from Moroccan biomass: Assessment of parameters' effect on CNC yields

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Biobased materials are advocated for their bioavailability, affordability, non-toxic attributes, and environmental friendliness. Consequently, harnessing plant biomass becomes pivotal in sustainable development endeavors, enabling the production of diverse high-value goods within the renewable energy and nanostructured carbon materials domains. Cellulose is the most abundant natural polymer in biomass, it is highly stable and can be isolated from a wide range of plant, algae and animal sources. Cellulosic nanomaterials (CNCs) are extracted using various techniques, exhibiting a crystalline structure with rigid rods hundreds of nanometers long and less than 100 nm in diameter [1]. These nanomaterials have remarkable properties compared with cellulose fibers, due to their manometric size, which gives them a high specific surface area, implying stronger interactions on the nanoparticle/matrix interface [2]. These nanoparticles can also be used as multi-purpose reinforcements in the automotive, packaging, and construction industries. This study's framework focuses on the extraction of nanocelluloses from Moroccan biomass. Recognized for their antioxidant, antimicrobial, and antifungal properties, aromatic medicinal plants (AMP) produce substantial residual biomass post-extraction, presenting an opportunity for CNC synthesis. Notably, within the rosemary essential oil industry, it's estimated that production processes yield approximately 10 to 20 kilotons of rosemary residues annually, highlighting the significant potential for resource recovery and sustainable materials production. Herein, initial experiments, focusing on isolating nanocellulose from rosemary, underscored the substantial impact of several parameters on the yield of nanocelluloses, including acid type and concentration, temperature, and contact time. The structural analysis of the obtained CNCs shows promising results, confirming the effectiveness of the extraction process employed.

Keywords: Biomass, Cellulose, Nanocelluloses, Extraction process, Acid treatment.

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C.A. 111

Fly ash valorization in a circular economy and environmental preservation perspective: challenges and opportunities

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Fly ash is a byproduct of thermal processes; specifically, it results from coal combustion in thermal power plants. Fly ash exhibits remarkable properties and could be effectively utilized in manufacturing new materials for a wide range of applications. Research on fly ash recovery, coupled with a reduction in landfill options, has spurred numerous programs in this direction, yielding promising results.

The uniqueness of the fly ash material in this study lies in its derivation from staged coal combustion, the first of its kind originating from an ultra-supercritical thermal power plant.

This study examines the challenges associated with fly ash handling. Physicochemical characterization employed X-ray diffraction (XRD), infrared spectroscopy (ATR), thermogravimetric analysis (ATG/ATD), scanning electron microscopy (SEM), moisture content (H), swelling index (GI), and porosity (P).

The study underscores the need for improved characterization and identification of fly ash, particularly through the development of a more detailed typology to effectively utilize qualitative and quantitative data. Furthermore, it advocates for regulatory framework adjustments and aims for greater harmonization to reassure producers.

Keywords: Waste recovery, Staged combustion, Fly ash ultra-supercritical power plant, Physicochemical Characterization.

C.A. 112

Effect of BMT compounds on the degradation of azo organic pollutants

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Most of the dyes produced by dyeing, painting and textile industries contain different organic contaminants, which are toxic and carcinogenic, and thus they have imposed a serious problem in environments [1]. Wastewaters from various industries, factories, laboratories, etc. are serious problems to the environment. The discharged wastes containing dyes are toxic to microorganisms, aquatic life and human beings [2]. Textile dyes and other industrial dyestuffs constitute one of the largest groups of organic compounds that represent an increasing environmental danger.

Degradation of dyes in industrial wastewaters has therefore received increasing attention and some methods of remediation have been proffered. Traditional physical techniques (adsorption on activated carbon, ultrafiltration, reverse osmosis, coagulation by chemical agents, ion exchange on synthetic adsorbent resins, etc.) have been used for the removal of dye pollutants [3,5]. To date, several photocatalysts have been explored in order to assess their photocatalytic efficiency against harmful pollutants in water and in the air. Titanium oxide TiO_2, which is a semiconductor with a band gap of around 3.2 eV [6] in width, is currently the most studied.

In this work, a new BMT composite was obtained by solid-state synthetic method. The quality of the crystalline phases was studied by X-ray diffraction, SEM and FTIR to determine the morphological and compositional properties off the powders. The degradation of different organic dyes by composites catalysts under UV irradiation was investigated. The photocatalytic results indicated that all the composites prepared exhibited higher photocatalytic activities.

Key words: Photocatalytic activity; dye; XRD; BMT powders.

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C. A. 113

Efficient detoxification of Cr(VI) from Aqueous Solution Using Polyaniline@ Phosphate Iron Oxide Composite

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In the pursuit of advancing environmental safety in water treatment, a novel composite Polyaniline@ Phosphate Iron Oxide, has been identified as a highly effective adsorbent for removing hexavalent chromium ions. Synthesized through an in situ chemical polymerization technique, this composite underwent characterization using various analytical methods, including X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), BET analysis for nitrogen adsorption-desorption isotherms, and scanning electron microscopy (SEM). Experimental optimization of parameters, such as pH, adsorbent dosage, contact time, initial Cr(VI) concentration, and coexisting ions confirmed the efficacy of Polyaniline@ Phosphate Iron Oxide as a proficient adsorbent for Cr(VI) in a synthetic solution. The increased efficiency of Cr(VI) adsorption at lower pH levels emphasizes the predominant role of electrostatic interactions in governing the binding mechanism of Cr(VI) to the surface of Polyaniline@ Phosphate Iron Oxide. The Freundlich model and the pseudo-second order kinetic model exhibit the strongest correlation with the experimental findings. Furthermore, the adsorption capacity of Cr(VI) onto the Polyaniline@ Phosphate Iron Oxide composite reached a maximum monolayer coverage of 682.30 mg g^{-1}. Consequently, the utilization of the Polyaniline@ Phosphate Iron Oxide composite for Cr(VI) adsorption showcases its potential to effectively purify wastewater at a large scale.

Keywords: Adsorption, composite, In Situ Chemical Polymerization, BET, SEM

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C. A. 114

Elaboration and characterization of LDH- Sulfonated Styrene hybrid for the removal of organic dye pollutants

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Layered Double Hydroxide (LDH) materials represent great interest in the industrial field due to their accessibility, ease of preparation and high surface activity at low cost. This type of materials offers a variety of applications in industry and the environment, such as anion exchange, catalysis, adsorption, and more [1-4].

In this work we focused on the intercalation of the sulfonated styrene (vinylbenzene sulfonate (VBS)) monomer in the ZnAl-LDH phase in order to improve the adsorption capacity of the latter in the aqueous medium. Then we studied the adsorption performance of the ZnAl-VBS material for the food colorants Tartrazine and Rouge Allura AC in aqueous solution.

Various parameters governing the adsorption capacity of the prepared adsorbent were optimized, i.e. temperature, contact time, initial dye concentration, solution pH, etc. Adsorption kinetics were studied by examining three kinetic models: pseudo-first-order, pseudo-second-order and the intra-particle diffusion model. Next, we present the results of adsorption equilibrium modeling using the Langmuir and Freundlich isotherm models. The thermodynamic parameters of adsorption have also been studied.

The results obtained show that the maximum adsorption capacities of the two dyes, TRT (416.7 mg/g) and RAAC (277.8 mg/g), are more efficient compared to other types of adsorbents. The adsorption isotherms are well described by the Langmuir model, and the kinetics modeling is governed by the pseudo-second-order model. The thermodynamic study indicates that the adsorption process for the two dyes is endothermic, favorable, and spontaneous.

Keywords: Hybrid Materials, Environment, Adsorption, Regeneration.

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C. A. 115

The substituted 1,2,4 triazoles as effective corrosion inhibitors in acidic media

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Thermodynamic and electrochemical techniques, XPS ... were used to investigate the behavior of synthesized compounds in protecting mild steel (MS) against corrosion in molar HCl solution. Electrochemical impedance spectroscopy (EIS) at 303K showed a significant increase in polarization resistance (Rp) from an initial $21.57\Omega\ cm^2$ to 271.6 and $470.4\ \Omega\ cm^2$, at optimal concentrations of Dy-H & Dy-CH3 respectively. This equated to inhibitory efficiency of 92.1% for Dy-H and 95.2% for Dy-CH3. Adsorption of inhibitor compounds causes a significant drop in effective double layer capacitance. The polarization measurement also indicated that these compounds are mixed inhibitors. The both inhibitors were adsorbed on the mild Steel in accordance with Langmuir adsorption model. X-ray photoelectron spectroscopy (XPS) was used to analyze the adsorbed layers on the MS surface. Based on the experimental results and theoretical calculations, the correlation of the electron properties with the adsorption and inhibition behavior of the both compounds was verified.

Keywords: Triazole derivatives, Electrochemical techniques, XPS analysis, Theoretical calculations

C. A. 116

Manufacturing activated carbons from biowaste: Utilization in adsorbing pharmaceutical molecules from wastewater

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This work discusses the fabrication of nanostructured carbons with enhanced porosity and functionality to be exploited in wastewater purification. The nanostructured carbons (NCs) were synthesized by subjecting flaxseed waste to a two-step process involving hydrothermal carbonization and H_3PO_4-chemical activation. The (NCs) were characterized employing a variety of analytical techniques such as scanning electron microscopy coupled with EDX, X-ray diffraction, FTIR spectroscopy, and N_2-sorption. The results indicated that the NCs possess excellent textural properties and surface functionality, and well-defined morphologies. The properties of these materials were then exploited to achieve remarkable adsorption capacities towards diclofenac sodium. These results highlight the potential of NCs to be used effectively for removing pharmaceutical pollutant from wastewater.

Keywords: Flaxseed waste, Phosphoric acid, Diclofenac sodium.

C.A. 117

Removal of an organic dye by adsorption and Fenton process on a support based on CuAl anionic clay

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A considerable quantity of reactive dyes finds extensive application across various sectors, including textile, printing, plastic, cosmetics, pharmaceuticals, and food industries (*1*, *2*). The resultant wastewater containing these dyes emerges as a significant environmental risk. When these dyes are released into aquatic systems without proper treatment, they pose a substantial threat to both aquatic and terrestrial plants and organisms (*3*).

Given the persistent expansion of these industries, it is imperative to explore cost-effective and efficient techniques for industrial wastewater treatment. Among these approaches are the processes of adsorption and Fenton degradation, which we apply in this work on an anionic clay of the CuAl type Woodwardite for the removal of the Reactive Yellow 145 dye.

The influence of various parameters such as the contact time, initial dye concentration, adsorbent material mass, and solution pH… on the adsorption and degradation process was investigated.

Keywords: Reactive Yellow 145, Anionic clay, Adsorption, Fenton process.

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C.A. 118

Efficiency of Textile Waste in Cationic Dye Removal: Experimental Insights

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Wastewater from the textile industry contains hazardous effluents with complex elements that, without proper treatment, adversely impact the environment, posing risks to aquatic ecosystems and human health. Over recent decades, a variety of cleaning and recovery methods, ranging from chemical to physical separation, have been employed. Compared to alternative techniques, adsorption has proven to be highly effective in removing impurities from wastewater.

This study focuses on treating industrial dyes using recycled waste from an industry in Morocco. The material was characterized using several methods; including Fourier transform infrared spectroscopy, scanning electron microscopy, fluorescence, and X-ray diffraction. The results indicate that the material is rich in hydroxide and carbon chains, exhibiting diverse and heterogeneous shapes.

The textile waste utilized in this study shows promising results in removing cationic dyes, with a discoloration percentage reaching up to 98% under experimental conditions. These findings suggest its potential as a cost-effective alternative to expensive industrial adsorbents, as well as natural materials and plants commonly used in pollutant adsorption.

Keywords: Adsorption technology, recycled waste, characterization methods, cationic dye removal.

C.A. 119

Fouling of reverse osmosis membranes during brackish water treatment: Membrane autopsy results

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The accumulation of solid deposits on membrane surfaces, a phenomenon known as fouling, has become one of the major challenges in seawater desalination. This problem reduces the service life of reverse osmosis modules, thus limiting their efficiency.

In this study, we examined membrane fouling during brackish water treatment. We collected data on operational performance and used advanced techniques to characterize fouling. To this end, we employed a reverse osmosis membrane unit and carried out in-depth analyses. The recovered foulants were subjected to various characterization methods such as Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray energy dispersive spectroscopy (EDS), X-ray fluorescence spectrometry (XRF) as well as thermogravimetric analysis and differential scanning calorimetry (TG/DSC).

The results show that fouling of membrane elements is mainly caused by adsorption and deposition of inorganic matter. They also underline the importance of carefully selecting the inhibitors used in the pretreatment system of the reverse osmosis treatment plant, based on their compatibility with the membrane structure. Finally, this study highlights the crucial importance of characterization to verify fouling mechanisms.

Keywords: Fouling; Reverse osmosis; Membrane; brackish water; Autopsy.

C.A. 120

Effect on the mechanical properties of ceramic bodies incorporating granite waste as sustainable raw materials - A review

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The recovery of industrial waste is an international issue. Several studies encourage the reuse of waste in order to protect the environment and to move towards an eco-responsible economy. Granite waste, as a highly polluting waste formed during the cutting operation of granite blocks, can be considered as a potential raw material in various fields, especially as building and construction materials and mainly in glassmaking and ceramics industries.

The objective of this work is to review the feasibility of using granite waste as a sustainable alternative for ceramic raw materials. Previous studies show that mixtures of granite waste with clay can produce ceramic bodies in agreement with the requirements of ceramic manufacturing standards. The materials are usually characterized by X-ray fluorescence spectroscopy, X-ray diffraction, scanning electron microscopy and the mechanical, strength and firing properties need to be tested.

The incorporation of granite waste into ceramics up to 40% by weight, at different firing temperatures, could confer mechanical strength and hardness to the body due to the molten glass phase formed by alkali feldspars. However, the rock formation conditions, chemical composition, porosity and grain size influence the material features.

Granite waste can be used as an eco- friendly raw material for ceramic bodies with a high strength and a satisfaction of standard requirements. Moreover, the reuse of this waste can mitigate both pollution and depleting natural resources.

Keywords: granite waste, alkali-feldspar, pollution, mechanical properties, ceramics bodies, Sustainability.

C.A. 121

Retention of methylene blue by a geopolymer based on red brick waste from an aqueous solution using an adsorption process

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Discharges of various micropollutants (organic and inorganic) into the environment are on the increase. These pollutants are generally toxic, poorly biodegradable, and cause numerous adverse health effects.

In this context, this work focuses on the development of a geopolymer based on red brick waste and the alkaline sodium silicate solution (Na2SiO3) and the sodium hydroxide solution (NaOH) of 12 mol/L are mixed with a mass ratio of 2.5, with a view to its application as an adsorbent in the treatment of an aqueous medium contaminated by methylene blue. The synthesized geopolymer was characterized by various analytical techniques. Adsorption tests were carried out by varying various parameters likely to affect adsorption performance, including adsorbent dose, solution pH, contact time, initial methylene blue concentration, and solution temperature.

The kinetic study revealed that the geopolymer eliminates methylene blue relatively quickly. The pseudo-second-order model is the most suitable for presenting the adsorption mechanism. The isotherm for methylene blue retention on geopolymer is in perfect agreement with the Langmuir model. Evaluation of the thermodynamic quantities showed that the methylene blue adsorption process is favorable, spontaneous, and endothermic. The results we have found allow us to predict that the use of these new generations of geopolymers offers great potential for the retention of cationic textile dyes.

Keywords: Adsorption; red brick waste; Geopolymer Beads; Methylene Blue.

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C.A. 122

A Sample Preparation Method for the determination of heavy metals with Inductively coupled plasma mass spectrometry (ICP-MS) in Cosmetics products

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The growing application usage of cosmetics by diverse populations has led to increase public health concerns due to the presence of heavy metals such as Hg, Pb, Cd, and As in cosmetic formulations as ingredients or impurities ,. These metals are discharged into the final product by metallic devices during the manufacturing process or through metallic containers used to package these cosmetics products [5 ,6]. Therefore, quality control measures should be enforced to ensure that metal concentrations in cosmetic products do not exceed regulatory limits. The aim of this study is to determine heavy metals in some locally available cosmetics products such, foundation cream,serum,mask,and sun's cream. The concentration of As, Pb,Cd,Hg, Cr, Ni, and Sb was determined in seven samples using Inductively Coupled Plasma Mass Spectroscopy (ICP-MS). The method used in this study is a quick and simple one, easy to implement, compared to other methods. The suitability of the method for the analysis of heavy metals was demonstrated by excellent recoveries ranging from 80–120% which indicating the reproducibility and the reliability of the analytical procedure.The method was also validated by the participation in three interlaboratory tests with acceptables z-scores ($-2 \leq z \leq 2$, and by the analysis of reference materials in one sample of cream and one of champoo Satisfactory results were found for all parametres which indicates that the method is robust and applicable for the analysis of heavy metals in a wide range of cosmetic products.

Keywords: cosmetic products, Heavy metal contamination, ICP-MS, consumers' health.

C. A. 123

Desalination Reverse Osmosis reject brine as a novel-based porous geopolymer for phosphate removal from contaminated media

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Desalination reverse osmosis reject brine-based porous geopolymer (RO/GP) was produced and investigated as an improved adsorbent for PO_4^{3-} removal from tainted seawater, brackish water, river water, and municipal wastewater effluent. The RO reject brine/geopolymer was produced by reacting metakaolin and fly ash with a Na-alkali activator and anhydrous RO brine as a sacrificial template. The influence of RO reject brine content on water absorption, porosity, mechanical, and structural properties were examined. The developed RO-based geopolymers exhibited the greatest porosity (58.3 - 84.2 % vol%), a significant ratio of open porosity to total porosity (67.7 – 92.1 %), and outstanding compression strength (3.6 - 10.4 MPa). The produced RO/GP structure has an adsorption capacity of 92.4 mg/g for PO_4^{3-}. The sequestration reaction of PO_4^{3-} by RO/GP is of pseudo-second-order kinetic behavior via Chi-squared (χ^2), RMSE, and correlation coefficient (R^2) values. Regarding their agreement with Langmuir's behavior, the PO_4^{3-} adsorption uptakes occur in homogeneous and monolayer states. The reaction is exothermic, spontaneous, and favorable. The RO/GP exhibits significant affinity for PO_4^{3-} co-existing with Cl^-, Na^+, SO_4^{2-}, K^+, HCO_3^-, and Ca^{2+}. The RO/GP shows high safety during the adsorption investigation, with a total cost of 0.32 $/kg-P.

Keywords: RO reject brine, porous agent, geopolymer, adsorption, phosphate removal.

C.A. 124

Oxidation of sulfate to sulfite in the presence of CuP and CuP/V (2-12 wt.% V_2O_5)

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The oxidation of sulfate to sulfite over vanadium oxide catalysts is an essential and priority reaction in many industrial and environmental processes, contributing to the production of higher quality products and environmental protection, namely the manufacture of sulfuric acid.

A series of $V_2O_5/Cu_3(PO_4)_2$ catalysts was prepared by impregnation of 2-12% by weight of V_2O_5. The catalysts obtained were characterized by X-ray diffraction (XRD), infrared spectroscopy (IR), thermo gravimetric analysis (TGA) and differential thermal analysis (DTA).and by the isopropanol decomposition reaction. This highly sensitive technique provided us with relevant information on the nature of the catalytic active sites (acid-base) of the phases dispersed on the support.

X-ray diffraction (XRD) and infrared spectroscopy (IR) results confirmed the presence of V_2O_5 on $Cu_3(PO_4)_2$. The isopropanol decomposition test showed the presence of a large number of acidic sites. The application of catalysts in the reaction to convert sulfites into sulfates gave very good promoter results.

Keywords: oxidation, sulfite, sulfate, V_2O_5, $Cu_3(PO_4)$, Isopropanol decomposition

C.A. 125

Investigation of Current Density, Supporting Electrolyte, and pH Effects in the Electrochemical Degradation of Orange G with a Novel BHP@Bi2O3-Based Anode

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In this study, we synthetised a bilayer consisting of $BaHPO_4$ (BHP) and Bi_2O_3 through the electrodeposition technique. The produced anode was subjected to characterization using cyclic voltammetry to clarify the deposition reactions. Following this, structural and morphological analyses were performed using X-ray diffraction and scanning electron microscopy with energy-dispersive X-ray spectroscopy. Additionally, UV-vis diffuse reflectance spectroscopy was employed to determine the bandgap energies of both semiconductors. The electrochemical degradation performance of the anode on the anionic dye Orange G (OG) was assessed. We explored the impact of applied current density, choice of supporting electrolyte, and solution pH on the bilayer's degradation efficiency. Notably, the bilayer demonstrated a remarkable degradation efficiency of 98% within a 20-minute timeframe at an OG concentration of 10 ppm. This effectiveness was corroborated through electrochemical measurements, including linear sweep voltammetry and electrochemical impedance spectroscopy. A degradation mechanism was proposed based on Mott-Schottky measurements and trap studies. Moreover, the anode exhibited notable stability and reproducibility, enduring through 11 degradation cycles.

Keywords: Electrodeposition; Thin films; BHP@Bi_2O_3; Electrochemical degradation; Environmental treatment.

C.A. 126

Green Synthesis, Characterization of Nickel (II) Oxide NiO Nanoparticles, Optical Properties, and their Photocatalytic Application

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In this report, a new facile and green approach for synthesizing nickel (II) oxide nanoparticles NiO-NPs was performed using the extract of the wild plant Herniaria hirsuta (H. hirsuta).

Different spectral methods were used for the characterization of the biosynthesized NiO-NPs, ultraviolet-visible (UV-Vis) spectroscopy gave a surface plasmon resonance (SPR) peak of NiO-NPs at 301 nm, the estimation of direct and indirect band gaps by Tauc method is 3.02 eV and 3.40 eV respectively; Fourier transform infrared (FTIR) spectral analysis revealed the groups responsible for the stability and synthesis of NiO NPs, and X-ray diffraction (XRD) study confirmed the crystallinity of NiO NPs determined using Scherrer's formula with a crystallinity size of 20.82 nm.

The kinetic and catalytic activity of NiO NPs was studied in the presence of visible light irradiation by degradation of methylene blue dye (MB) and rhodamine B (Rh B).

Keywords: Nickel oxide nanoparticles NiO-NPs; Herniaria Hirsuta plant extract; Nickel nitrate Ni(NO3)2; Dye degradation; blue methylene; rhodamine B.

C.A. 127

Iron Spinel Oxides Based OER and ORR Electrocatalysts for Metal-Air Batteries Application

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In recent years, it has become increasingly urgent to find alternatives to lithium-ion batteries due to their limited energy density, limited lithium resources, and safety issues; hence hindering their further development. Rechargeable metal-air batteries (RMAB) have emerged as next-generation energy conversion and storage devices due to their high theoretical energy density. However, developing low-cost, earth-abundant, and efficient bifunctional electrocatalysts remains challenging, due to the slow electrochemical kinetics that trigger the ORR (discharge) and OER (charge) of RMAB, consequently limiting the overall efficiency of energy conversion. In this work, Cu substituted iron-based spinel oxides were prepared by a simple sol-gel synthesis method. The morphologic structure and crystallinity of synthesized powders were investigated using Scanning Electronic Microscopy and X-ray diffraction. The electrochemical performances against both OER and ORR were conducted on glassy carbon electrode (GCE) drop casted with metal oxide particles suspension. Preliminary results show satisfactory performance in terms of OER in alkaline media.

Keywords: Metal-Air Batteries, bifunctional electrocatalysts, energy density, sol-gel, OER, ORR

C.A. 128

Development of a green and renewable catalyst based on biopolymer for the synthesis of organic compounds

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In this study, we developed a green and renewable biopolymer-based catalyst for the synthesis of organic compounds. The increasing demand for organic chemicals has been accompanied by a growing awareness of the environmental problems associated with traditional catalysts. The solid biopolymer catalyst, derived from renewable sources, has been used for the synthesis of organic compounds. An in-depth analysis of the catalyst structure was carried out using techniques such as Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-Ray (EDX), Scanning Electron Microscopy (SEM) and Diffraction X-Ray (DXR), highlighting the amorphous structure of the catalyst as well as the complex interaction between the metal and the biopolymer functional groups responsible for its catalytic activity.

This catalyst can be easily recovered from the reaction mixture by filtration and reused at least five times without any reduction in its catalytic activity. The metal-biopolymer catalyst obtained, as a heterogeneous catalyst, showed exceptional catalytic activity, enabling organic reactions to be accelerated compared with non-catalyzed reactions, and in considerably shorter reaction times.

Key words: Green catalyst, Biopolymer, organic reactions, heterogeneous catalyst, Metal-biopolymer.

C.A. 129

Development of low cost Catalysts for Hydrogen Peroxide Decomposition for Space Propulsion Applications

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This research aims to address a major challenge in the field of space propulsion: the search for non-toxic and effective alternatives to hydrazine, considered as a conventional propellant for the reaction control system (RCS) of satellites. Table [1] illustrates comparative data on the toxicity of hydrazine and hydrogen peroxide (H_2O_2) as a potential eco-friendly alternative for this application. Thus, H_2O_2 is a promising green propellant with interesting advantages such as non-toxicity, availability, transportability, and high energy efficiency. Moreover, effective catalysts are essential to harness the potential of H_2O_2. Meanwhile, the aim of this investigation is to evaluate two catalysts composed of copper (Cu) impregnated on a silica (SiO_2) support for the purpose of catalyzing the decomposition of H_2O_2. The catalysts were synthesized with 5% and 10% compositions of Cu. The primary objective is to compare the effectiveness of these two catalysts when utilized in the decomposition reaction of H_2O_2. To achieve this goal, we established an experimental setup to measure the pressure difference between a vial representing catalytic decomposition and another vial representing spontaneous decomposition, all at a constant temperature. Additionally, analytical techniques such as XRD (X-ray Diffraction) and FTIR (Fourier Transform Infrared Spectroscopy) were employed to characterize in detail the structure and properties of the catalysts. This comprehensive understanding will contribute to advancing the development of more efficient and environmentally friendly catalysts for space propulsion applications. Our research aligns with a perspective aimed at making space exploration more sustainable and reducing the environmental impact of space travel.

Table 1. R-phrase categories for hydrogen peroxide and hydrazine.

R-Values	H_2O_2	Hydrazine
R23-28	**0**	**1**
R39	**0**	**0**
R48-68	**0**	**0**
R45-49	**0**	**1**
R46	**0**	**0**
R60-61	**0**	**1**
R50-53	**0**	**0**
R54-59	**0**	**0**

R-phrases (Risk phrases), as established by European Union Directive: R23 through to R28: toxic in contact or if swallowed.
R45, R49: carcinogen categories 1 and 2.
R60: may impair fertility.
R61: may cause harm to the unborn child[1].

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C.A. 130

Development of new catalytic materials for liquid effluent disposal

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Titanium dioxide (TiO_2) is a well-known material due to its important applications in photocatalysis, and in various environmental fields [1-2], However, major drawbacks, such as low surface area and high band gap, have often limited TiO_2 materials for suitable applications. Self-assembled TiO_2 nanostructured materials with well-defined spherical morphologies have been synthesized using a biopolymer, sodium alginate, as a template, providing porous structures and controlling the morphology of TiO_2 nanoparticles under different synthesis conditions [3]. X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) and energy dispersive X-ray spectroscopy (EDS) techniques were used to characterize TiO_2 nanoparticles. N_2 sorption analysis revealed moderately good surface area. The BET surface areas of pure TiO_2, TiO_2 with polymer (Tp=60°C) samples were (55.5851 m²/g), (65.0787 m²/g) respectively. Zero charge point (PZC) analysis revealed the zero-charge point (PZC) of pure TiO_2 is at a pH of about 6 and the zero-charge point (PZC) for modified TiO2 nanoparticles is at a pH of about 10.

Keywords: Self-assembly of nanoparticles, biopolymer templating, mesoporous materials, TiO_2

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C.A. 131

Immobilization of Cobalt oxide onto mesoporous activated carbon for peroxymonosulfate activation

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This study describes an efficient methodology for preparing cobalt-based catalysts (Co(X%)@AC) to be used for removing diclofenac from polluted water via advanced oxidation processes. Mesoporous activated carbon was derived from argan nut shells through a two-step process involving hydrothermal carbonization and chemical activation. Cobalt nanoparticles were then immobilized onto the activated carbon using the wet impregnation method, utilizing $Co(NO_3)_2 \cdot 6H_2O$ as the cobalt precursor. The cobalt (Co) weight loadings in the total catalyst amount were 0.4%, 1%, 2%, and 5%. The catalysts were characterized employing SEM-EDX, XPS, FTIR, N_2-physisorption, and XRD techniques. The catalytic activities of the Co(X%)@AC-peroxomonosulfate systems were systematically assessed for the degradation of Diclofenac sodium (DCF) in an aqueous medium. The study investigated the effects of experimental parameters, including Co-mass loading, peroxomonosulfate concentrations, and solution pH. The results demonstrated the effectiveness of Co(X%)@AC in activating peroxomonosulfate and degrading DCF, achieving an excellent DCF degradation and total organic carbon removal efficiency of 98% and 76%, respectively.

Keywords: Biomass, mesoporous Carbon, Water treatment, Diclofenac, Advanced oxidation process; Peroxymonosulfat

C.A. 132

Facile fabrication of ZnO/Hydroxyapatite nanocomposites for enhanced photocatalytic performance

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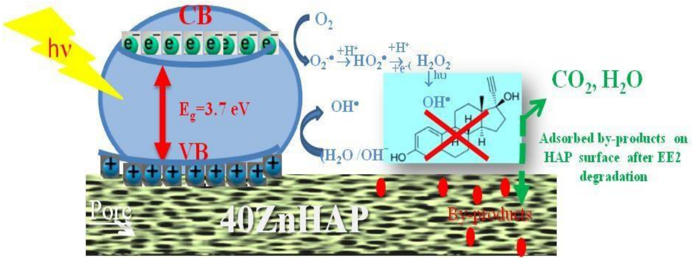
The development of active, stable and efficient porous materials is necessary for the photodegradation of persistent organic pollutants. To address this challenge, we proposed to synthesize binary ZnO/hydroxyapatite nanocomposites for efficient photocatalytic application. The structural and textural characteristics of the prepared nanocomposites were determined by FT-IR, XRD, TEM/EDX, chemical analyses, diffuse UV-Vis spectroscopy, and BET surface analysis. The obtained results showed successful fabrication of synthesized nanocomposites with improved specific surface area. The photocatalytic efficiency of the nanostructures on some toxic organic species and the antibacterial activity against pathogenic strains were studied. Zn/HAP photocatalysts demonstrated considerable adsorption rate and exceptionally enhanced photocatalytic activity on the degradation efficiency of drugs and dyes. The proposed photocatalytic mechanism illustrates the electron transfer facilitated by the nanocomposite structure that results in spatial separation of electron–hole pairs. Compared with ZnO and HAP, the prepared ZnO/HAP binary nanocomposite showed good photocatalytic degradation under the action of UV illumination, good efficiency and good trapping of by-products. A good stability of the photocatalysts was obtained with conservation of the catalytic activity which does not exceed 10% in the fifth cycle.



Schematic diagram of the photodegradation mechanism of EE2 by porous 40ZnHAP nanocomposite showing the process of excitation and transfer of charge carriers in the nanocomposite.

C.A. 133

A comparative study of new type of $BiPO_4$ with TiO_2, ZnO and Bi_2O_3 catalysts for the photocatalytic degradation of Rhodamine B: kinetics and mechanism of photodegradation

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The main objective of this study was to evaluate the photocatalytic efficiency of $BiPO_4$ (BiP) particles, in aqueous solution of rhodamine B (RhB). The monoclinic $BiPO_4$ polycrystalline phase with space group $P2_1/n$ was synthesized by a solid-state reaction with heat treatment at 500 °C in air for 3h. The BiP crystal structure was characterized by X-ray diffraction (XRD). Scanning electron microscopy (SEM) coupled with energy dispersive X-Ray analysis (EDX) showed the presence of submicronic regular faceted crystallites. Fourier transform infrared (FTIR) and Raman spectroscopy allowed characterizing the functional groups in the monoclinic structure. The photodegradation of RhB, reacting in presence of the as synthesized BiP particles, was studied as a function of time from the variation of the RhB absorption band at 554 nm. The photodegradation efficiencies of BiP, TiO_2, ZnO and Bi_2O_3 particles were compared through the determination of apparent rates constants showing that these BiP submicronic particles presented the highest performance. Using a series of analytical techniques (UV-Visible spectrometry, high-performance liquid chromatography and liquid chromatography coupled with Mass Spectrometry, total organic carbon), a detailed photocatalytic degradation mechanism of rhodamine B was proposed, and the mineralization of rhodamine B was confirmed.

Keywords: $BiPO_4$; solid-state reaction; photocatalytic efficiency; Rhodamine B; mineralization and photodegradation mechanism.

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C.A. 134

Efficient removal of Organic Pollutants via catalytic wet peroxide oxidation over Clay-Based Catalysts

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Efficient removal of organic pollutants from wastewater is imperative for environmental remediation. Catalytic wet peroxide oxidation (CWPO) has emerged as a promising method due to its ability to degrade various organic compounds effectively. In this study, we investigate the application of CWPO using clay-based catalysts for organic pollutant removal [1-4]. The process involves activating hydrogen peroxide with clay-based catalysts to generate highly reactive hydroxyl radicals, which oxidize organic contaminants into harmless byproducts. Our synthesized catalysts demonstrated excellent catalytic affinity towards the degradation and mineralization of three model contaminants of emerging concern: 4-Nitrophenol (4-NP), Methyl Orange (MO), and Amoxicillin (AMO).

Under optimized conditions, complete removal of contaminants was achieved after 2 hours of oxidation, with substantial reductions in total organic carbon (TOC) levels. Specifically, TOC reductions of 42%, 47%, and 56% were observed for 4-NP, MO, and AMO, respectively. Furthermore, elucidation of the oxidation reaction pathways was performed through LC-MS analysis, which identified intermediates and byproducts. The stability of the synthesized materials was assessed using X-ray Photoelectron Spectroscopy. Overall, our findings highlight the effectiveness of CWPO with clay-based catalysts for efficient organic pollutant removal from wastewater, offering promising prospects for environmental remediation.

Keywords: Organic pollutants; Clays; Catalysts; CWPO; wastewater treatment.

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C.A. 135

Templates effect on morphology and photocatalytic properties of ZnO nanostructures using precipitation method: A DFT perspective

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The aim of this work is to synthesize zinc oxide in the presence of Chitosan [1] and Pluronic 123 [2] as templates and to conduct a comparison of their optical and morphological properties in the prepared materials, along with a photocatalytic study. The resulting nanoparticles were analyzed using various techniques, including XRD, FTIR, UV/Vis, EDX, SEM, and N_2 adsorption-desorption. Furthermore, the interactions between the photocatalyst and the organic dye were explored through DFT calculations. The material synthesized via chitosan showed a lower band gap. The morphology of the oxides was altered by using different templates; the use of chitosan resulted in irregular particles with a smaller size compared to the use of a surfactant (P123). N_2 adsorption-desorption analysis showed that the use of chitosan as a directing agent gave the highest specific surface area (SSA), which is 20.57 m^2/g. Moreover; both materials revealed high stability and significant photocatalytic activity at solution pH (without adjustment) under UV-B radiation.

Key words: Biopolymer, surfactant, photocatalyst, organic dye, DFT.

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C.A. 136

Formulation, characterization, and study of the physical and mechanical properties of organic/inorganic composite geopolymer binders

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Geopolymers are innovative materials based on the reaction between an aluminosilicate source such as fly ash or clays and an alkaline solution. They offer numerous possibilities in terms of formulation, characterization, and study of physicochemical properties. In this research work, the focus is on the formulation and study of the properties of organic/inorganic composite geopolymers. The characterization of raw materials and synthesized geopolymers was carried out using X-ray diffraction (XRD), X-ray fluorescence (XRF), and Fourier-transform infrared spectroscopy (FTIR). The study of physicochemical properties of organic/inorganic composite geopolymers includes the measurement of parameters such as mechanical strength and density. These properties are influenced by the type of organic and inorganic additives in the formulation of geopolymers. The synthesized geopolymers GP-CV were applied in the field of environment for the adsorption of a dye (crystal violet). The experimental study was conducted in batch mode, and various experimental variables were analyzed, such as contact time, adsorbent mass and initial dye concentration. The evaluation of experimental parameters using different types of isotherms showed that the adsorption process was adequately described by the Langmuir model. The study of kinetic models revealed that the pseudo-second order model best described the adsorption mechanism. This research aims to formulate, study, and optimize the properties of organic/inorganic composite geopolymers. The objective is to obtain high-quality geopolymers and apply them in wastewater treatment while valorizing industrial waste and by-products.

Keywords: geopolymers, aluminosilicate-alkaline reaction, formulation, characterization, mechanical properties, organic/inorganic composite geopolymers, environment, wastewater treatment, adsorption, crystal violet.

C.A. 137

Hysteresis behaviors of a graphene bilayer with mixed spins (5/2, 1/2): Monte Carlo simulations

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Using Monte Carlo simulation, we have studied the hysteresis behaviour of a mixed-spin (5/2, 1/2) ferromagnetic graphene bilayer. The effects of exchange interactions, crystal field and temperature on the hysteresis loops, the coercivity and the remanence of the system are studied for certain physical parameters. As a function of certain Hamiltonian interactions, the multiple hysteresis behavior is observed.

Keywords: Graphene bilayer, Monte Carlo simulation, Hysteresis loops, remanence, coercivity

C.A. 138

Theoretical Study of Diels-Alder Cycloaddition Reactions and Evaluation of Biological Activity of the Obtained Derivatives

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In the context of this work, we present a theoretical study on the reaction of substituted dipoles with various dipolarophiles. For this purpose, we employed the DFT [1] (Density Functional Theory) quantum method and the B3LYP hybrid functional [2], which provide a good description of a number of physico-chemical parameters. The application of frontier orbital theory and conceptual DFT allowed us to determine the nature of these reactions and calculate various global and local reactivity indices. The complete optimization of the different stationary points involved in each reaction was performed, and vibrational calculations showed that the reactants and products are minima on the potential energy surface, with the transition state exhibiting a single imaginary frequency. Similarly, calculations of different energy levels and thermodynamic parameters allowed us to plot the energy profile for the different reactions and provide an interpretation of the kinetics of the studied reactions. The theoretical results obtained indicate that these different reactions follow a non-concerted mechanism for the various dienes and dienophiles studied.

Keywords: Diels-Alder Reactions, DFT Calculation

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C.A. 139

Simulation and Optimization of Sulfuric Acid Production: A Chemical Process Engineering Approach

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Sulfuric acid (H2SO4) is one of the largest-volume industrial chemicals produced in the world, and indeed, a nation's H2SO4 production is a good indicator of its industrial strength. The major end-use market for H2SO4 is the production of phosphate fertiliser materials [1]. This compound is furthermore used in the production of a wide variety of chemicals, in the metal processing industry, as an electrolyte in the lead-acid batteries that are used in automobiles, and in the petroleum refining industry to remove impurities from gasoline and other refinery products. The main purpose of the study is to simulate and optimize the annual profit 99.4% sulfuric acid plant by a softwar program used for chemical processsimulation. In this project, a simplified sulfuric acid production process is simulated and optimized [2]. The figure below describes the steps of the adopted sulfuric acid production process.

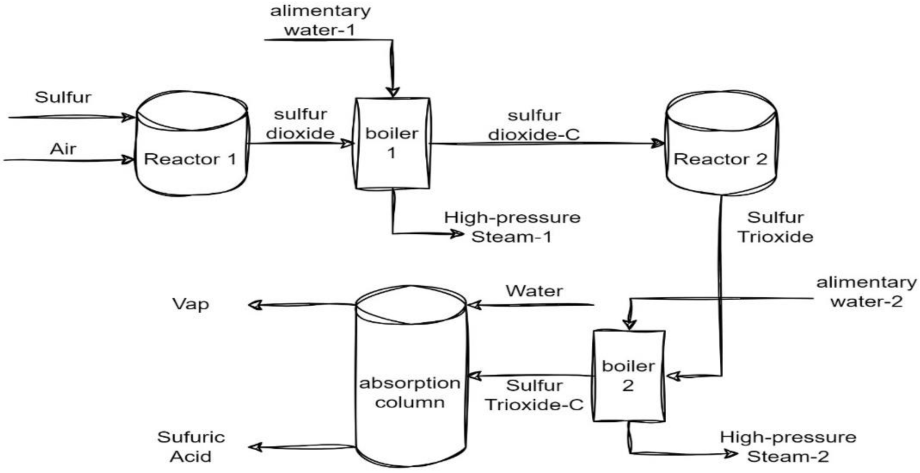

Figure 1. Flowsheet of sulfuric Acid production process

Keywords: Simulation, Optimization process, Engineering approach, Sulfuric acid production.

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C. A. 140
MCNP6.2 simulation to study GAGG(Ce) scintillator for Gamma-ray detection

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Inorganic scintillator is a kind of luminescent materials which is able to absorb and convert high ionizing radiation such as X and gamma-ray by emitting ultra-violet or visible photons. A scintillation detector composed by a scintillator crystal with a photodetector is widely used in high energy physics, non-destructive testing and nuclear medicine….etc. Among these scintillators Cerium-doped Gadolinium Aluminum Gallium Garnet (GAGG:Ce) is one of the promising materials [1,2]. In fact, it has high density, high light yield and fast decay time which are suitable for radiations detection [3]. For its excellent properties it has gained recently attention for its potential applications in medical imaging [4] including positron emission tomography (PET), single photon emission computed tomography (SPECT) and computed tomography (CT).

In this work, we propose to investigate the response of the $RE_3(Al, Ga)_5O_{12}$ (RE = Y, Gd, Lu) referred as multicomponent garnet scintillators [5], with MCNP6.2 simulation code based on the Monte Carlo method to the gamma rays of energy between 60 keV and 1442 keV. The parameters studied are the energy resolution and the detection efficiency which are decisive characteristics in the performance of the detector.

Keywords: Scintillator, Energy efficiency, rare earth doping, radiation detection

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C. A. 141

Advancing Solid-State Hydrogen Storage: Exploring Al, Li, and Mg Based Materials and Clusters Using DFT Method for Enhanced Capacity and Kinetics

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This study focuses on exploring the properties of materials and clusters composed of Al, Li, and Mg to enhance solid-state hydrogen storage, with a primary emphasis on improving storage capacity, kinetics, and reversibility. The research encompasses material selection, structural and electronic studies, as well as the mechanism of hydrogen absorption/desorption. Thorough analysis of the thermodynamics and reversibility of the storage process is conducted. Computational models, including Density Functional Theory (DFT), are employed for a comprehensive understanding of the electronic structure and energetics of the materials. Anticipated outcomes include the identification of promising materials, insights into factors influencing kinetics and reversibility, and contributions to the development of efficient hydrogen storage systems. This work aligns with the broader goal of advancing clean energy technologies by addressing challenges in hydrogen storage for sustainable applications.

C. A. 142

Computational study and predictive investigation of the inhibitory behavior of Geranium essential oil: DFT calculation, Monte Carlo simulation and POM analyses

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This research investigates the potential of Geranium essential oil, a highly valued ingredient in the perfume and cosmetic sectors, as an environmentally corrosion inhibitor. The study specifically examines Rose-scented geraniums (Pelargonium species), which are cultivated in various regions such as Reunion, China, Egypt, Morocco, and India to produce "geranium oil". The present work aims to apply a computational investigation on the all of molecules that constitute the Geranium essential oil in order to predict the mechanism of inhibition, its adsorption on the metal and the key molecule of the inhibitory effectiveness. To accelerate the discovery and development of this essential oil as green inhibitor for steel, we started our predictive study with the calculations of the quantum parameters by applying the density functional theory (DFT). Then, we performed the Monte Carlo simulation to confirm and complement the results found through our study. Finally, we calculated the Petra/Osiris/Molinspiration analyses to predict properties, toxicity, drug-likeness and Bioactivity of all the molecules that constitute the Geranium essential oil. Finally, it was concluded that the Viridiflorin molecule is the key molecule which may be responsible for the inhibitory effect of Geranium oil.

Keywords: DFT, green corrosion inhibitor, Monte Carlo simulation, Petra/Osiris/Molinspiration Analyses

C. A. 143

Utilization of Thermochemical calculations in the elaboration of new materials

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This article highlights the significance of chemical equilibrium in understanding and calculating theoretical thermodynamic properties of chemical systems. The ability to predict these properties has widespread applications in both chemistry and chemical engineering. Over the past few decades, thermodynamic methods and calculations have become crucial tools for analyzing various processes and contributing to the development of new technologies.

The applications of thermodynamic methods extend to addressing contemporary challenges, such as meeting energy needs, optimizing the utilization of raw material resources, and implementing measures for pollution prevention and environmental protection. The article emphasizes that these endeavors cannot be effectively pursued without preliminary analyses based on well-established thermodynamic models. Specifically, thermochemical calculations play a vital role in the analysis of diverse processes and contribute to the creation of novel materials and technologies. The integration of thermodynamic principles into these analyses provides a foundation for making informed decisions in fields ranging from energy production to environmental conservation. Overall, the article underscores the pervasive influence of thermodynamics in advancing scientific understanding and technological innovation within the realms of chemistry and chemical engineering.

In this study, we explore the application of thermochemical calculations using HSC Chemistry software in the development of new materials. Three cases are examined: the thermal decomposition of $FeSO_4 \cdot 7H_2O$, the hydration mechanism of MgO-Cr_2O_3-Fe_2O_3 refractory bricks, and the Chemical Vapor Transport (C.V.T) of $Fe_2(SO_4)_3$ with HCl.

In summary, this study utilizes thermochemical calculations to deepen understanding in the thermal decomposition, hydration of refractory bricks, and chemical vapor transport, providing insights into the development of novel materials.

Keywords: Thermochemical Calculations, HSC Chemistry Software, Thermal Decomposition MgO-Cr_2O_3-Fe_2O_3, Refractory Bricks, Chemical Vapor Transport (C.V.T).

C. A. 144

Two-dimensional Dirac $Zr\mathrm{B}_2\mathrm{C}_2$ as a potential anode material for alkali metal-based batteries

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Finding an appropriate material for the anode in non-lithium-ion batteries is a considerable challenge. The task of crafting anode materials with enduring stability, substantial capacity, minimal diffusion obstacles, and exceptional cyclability is pivotal for propelling the battery industry forward.

We investigate the potential of a promising 2D anode material called $Zr\mathrm{B}_2\mathrm{C}_2$ using first-principles prediction. Our findings reveal that this material demonstrates thermodynamic, dynamic, and thermal stability, suggesting feasibility for experimental synthesis. It is found that the $Zr\mathrm{B}_2\mathrm{C}_2$ monolayer shows negative adsorption energies of - 1.87, - 1.68 and - 2.08 eV for Li, Na and K, respectively. More importantly, the alkali metal atoms show high diffusivities on the $Zr\mathrm{B}_2\mathrm{C}_2$ monolayer, with low activation energy. The calculated energy barriers along the migration paths are estimated respectively to be 0.586 eV for Li as well as to be 0.32 eV for Na, and to be 0.201 eV for K. Moreover, $Zr\mathrm{B}_2\mathrm{C}_2$ exhibits good ionic and electronic conductivity, suitable voltage profile, and high structural stability during the charge/discharge process.

The above-mentioned results suggest that the $Zr\mathrm{B}_2\mathrm{C}_2$ monolayer is a promising anode material not only for Li-ion and K-ion batteries, but also for other lithium-based and potassium-based batteries.

C. A. 145

Optimizing Optoelectronics Properties of Triphenylamine-Based Donor Materials for High-Performance Organic Solar Cells

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The global energy landscape is undergoing a profound transformation, driven by the urgent need to address environmental concerns and energy security. In recent years, there has been growing interest and investment in alternative solar energy technologies, with organic solar cells (OSCs) emerging as a promising candidate. OSCs offer several advantages over traditional silicon-based solar cells. In this investigation, a series of four donor materials (M1-M4) incorporating triphenylamine with a donor-acceptor-acceptor (D-A-A) configuration were developed. The electronic and optical properties of molecules M1-M4 and reference molecule TPA-R were explored through theoretical analysis using density functional theory (DFT) simulations at the B3LYP/def2-SVP and CAM-B3LYP/6-31(d,p) level of theory, respectively. The theoretical findings were subsequently compared to experimental data, revealing a high degree of agreement. All designed compounds, M1-M4, demonstrated prominent and extensive absorption peaks within the visible spectrum, ranging from 595 nm to 726 nm with comparatively narrower HOMO-LUMO energy gaps in comparison to the reference compound TPA-R. Analysis of the excited state reveals that all designed molecules exhibit a significantly elevated rate of electron-hole transfer (84%) from the donor moiety to the secondary acceptor group, which indicates that the modification of the first acceptor enhances the charge transfer properties. In summary, these findings present a promising opportunity for conducting further experiments aimed at synthesizing these molecules for potential application in organic solar cell devices.

Keywords: Organics Solar cells, DFT, TD-DFT, Charge Transfer, Triphenylamine

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C. A. 146

Combined 3D-QSAR and molecular docking study on alkylpiperazine derivatives to understand the binding mechanism of glycogen synthase kinase-3β inhibitors

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Glycogen synthase kinase-3β (GSK-3β), a protein kinase with diverse roles in various biological processes, has emerged as a promising target for drug research in the treatment of numerous clinical diseases. In this study, we employed a combination of computational techniques, including molecular docking and three-dimensional quantitative structure-activity relationship (3D-QSAR), to investigate a set of 36 alkylpiperazine derivatives as potential GSK-3β inhibitors. Our best-performing 3D-QSAR model yielded impressive conventional determination coefficients R^2 of 0.95 and leave-one-out cross-validation Q^2 of 0.56, showcasing its robustness and predictive capability. External validation using a test set of six compounds further confirmed the model's reliability, with anticipated R^2_{test} values of 0.87. To reinforce the validity of our 3D-QSAR model, a Y-Randomization test was conducted. Additionally, we carried out molecular docking simulations to explore the binding interactions between the most active compound and the active site of the GSK-3β protein (PDB ID: **1Q4L**). These docking results not only corroborated the findings from our 3D-QSAR analysis but also provided valuable insights into the binding mode of alkylpiperazine derivatives with GSK-3β. These compelling results not only enhance our understanding of how alkylpiperazine compounds interact with GSK-3β but also offer valuable information for the design and development of novel and potent GSK-3β inhibitors with potential therapeutic applications in various clinical diseases.

Keywords: GSK-3β; alkylpiperazine; derivatives; 3D-QSAR; CoMFA; molecular docking.

C. A. 147

Numerical investigation of the novel lead-free and eco-friendly $InSnCl_3$-based inorganic perovskite solar cell using SCAPS-1D device simulation

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Recently, there have been notable advancements in perovskite solar cells (PSCs), especially those incorporating organic-inorganic lead halides, leading to an impressive efficiency milestone of 25.20%. Nevertheless, the enduring problem of lead toxicity represents a substantial hurdle to their broad commercial utilization. In response to this challenge, the study centers on refining lead-free tin-based halide perovskite solar cells by employing SCAPS-1D simulation software for optimization. In our study, we use $InSnCl_3$ as the absorber layer, TiO_2 as the electron transport layer (ETL), PH3T as the hole transport layer (HTL), and various metals as the back metal contact. Thorough investigations have been conducted into various factors affecting device parameters, including thickness, doping concentration N_A, defect density, series and shunt resistance, operating temperature. Optimizing the back metal contact results in the formation of the $FTO/TiO_2/InSnCl_3/PH3T/Co$ structure. The optimized device exhibited a power conversion efficiency (PCE) of 16.26%, fill factor (FF) of 69.28%, a photocurrent density (Jsc) of 33.17 mA. cm^{-2}, a voltage open circuit (V_{oc}) of 0.7 V, and quantum efficiency (QE) of 100% in the visible range. This study demonstrates the potential of $InSnCl_3$ as a perovskite material to achieve toxicity free renewable energy.

Keywords: $InSnCl_3$ perovskite; SCAPS-1D; Eco-friendly; doping concentration; Defect density; Optimization.

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C.A. 148

Investigating the Reaction of (R)-Limonene with S-Thioacids Using Molecular Electron Density Theory

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The naturally occurring terpene limonene is widely distributed in nature. Specifically, (R)-limonene, the most abundant enantiomer, is found in the essential oils of lemons, oranges, and other citrus fruits, while (S)-limonene is present in peppermint and the racemate is found in turpentine. The reaction of (R)-limonene with S-thioacetic or S-thiobenzoic acid in toluene was investigated using molecular electron density theory methods at the B3LYP/6-311+G(d,p) level of theory. An analysis of global reactivity indices and the relative energies associated with different reaction pathways revealed that the reactions of (R)-limonene with thioacids are regioselective. Furthermore, topological analysis of the electron localization function of the most favored reactive pathways allowed for characterization of the reaction mechanism. Additionally, a docking study was performed on potential products tested against three human pathogenic bacteria: Bacillus subtilis, Escherichia coli O157:H7, and Proteus mirabilis.

Keywords: limonene; Regioselectivity; ELF; DFT.

C.A. 149

Unveiling the mechanism, regiochemistry, and solvent effects in the [3 + 2] cycloaddition reactions of nitrones to activated alkynes: A Molecular Electron Density Theory Perspective

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In this investigation, the [3+2] cycloaddition (32CA) reactions involving nitrone and acetylene derivatives 4b, 5b, and 6b were explored using Molecular Electron Density Theory (MEDT) and Density Functional Theory (DFT) methods at the B3LYP-D3/6 31G (d) computational level. The zwitterionic (zw-type) nature of these reactions was unveiled, demonstrating a one-step mechanism with activation enthalpies ranging from 8.80 to 14.37 kcal mol−1 in acetonitrile and ethanol solvents. While the reaction with (4b) produced two regioisomeric pathways leading to products P1,5-4b and P1,4-4b, reactions with (5b) and (6b) resulted in the formation of a single product. Topological analysis categorized the nitrone as a zwitterionic three-atom component (TAC), and conceptual density functional theory (CDFT) indices classified the 32CA reactions as forward electron density flux (FEDF) reactions. Further insights from Bond Evolution Theory (BET) indicated that the formation of new C-C and C-O covalent bonds did not initiate in the transition states but occurred in intermediate stages displaying pseudoradical centers of atoms already engaged in bonding.

Keywords: 4-isoxazoline, DFT/B3LYP-D3, regioselectivity, cycloaddition reaction, MEDT, ELF.

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C.A. 150

3D simulation of Polar Bear Fur's thermal Insulation

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The world has experienced a strong demand for energy in recent years, mainly due to the population increase and industrial processes requiring more power. In this context, thermal insulation can present an alternative to reduce excessive energy consumption in different areas (cooling, heating, etc.). Therefore, it is imperative to use sustainable construction techniques for more energy-efficient structures. Heat losses can be minimized by adopting a strategy similar to how living things naturally adapt to their surroundings.

The polar bear, an iconic animal of the Arctic, is remarkable for its size, strength, and capacity to withstand bitterly cold climates. One of the secrets to his survival is the fur. Upon accomplishing the 1D and 2D simulation of polar bear hair, we generated a 3D model of the hair within a 3D environment. Enhancing the design of insulating materials inspired by the properties of bear hair will be possible with a more realistic and detailed view of the hair, which is essential to comprehend their structure and organization. The energy efficiency of structures and machinery may be improved using these materials. Thus, the orientation of the bear's hair to the sun determines how much its skin temperature varies depending on which sections of its body are exposed to air and which ones are not.

We used MATLAB to develop a basic computer model of a hot and cold thermostat, symbolizing the animal's frozen outside and heated body. We integrated bear hair into tiny layers. Next, we examined the simulation's outcomes and adjusted the model's parameters to investigate the constructed model's radiative heat loss.

Keywords: Biophotonic, Bio-Inspiration, Radiative Transfer, Thermal Insulation, Polar Bear, Matlab, Diffraction.

C.A. 151

Theoretical investigation and analysis of self-assembly with [7]TH-CA molecules

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The self-assembly of organic molecules on metal surfaces holds great potential for developing nanomaterials with unique characteristics. Recently, structural and electronic properties of large self-assembled domains of [7]thiaheterohelicene-2,13-carboxaldehyde ([7]TH-CA) on Au(111) surface have been characterized by scanning tunneling microscopy (STM) experiments. In this work, we describe with numerical methods the adsorption state and interaction type of the molecular structures on Au(111) under the same tunneling conditions.

The theoretical investigations have been carried out with an extended semi-empirical atom superposition and electron delocalization (ASED+, Atom Superposition and Electron Delocalization) based on the extended Hückel molecular orbital theory. Calculated STM images were obtained within the EHMO-ESQC method (Extended Hückel Molecular Orbital-Elastic-Scattering Quantum Chemistry), which describes the electronic scattering between the substrate and the tip by modeling the chemical structure of the tunnel gap (substrate, molecule, tip apex, and tip substrate).

On the substrate, [7]thiaheterohelicene-2,13-carboxaldehyde molecules self-organize in extended 2D structures that appear to be composed of alternating P and M enantiomers; chains connected together through Vander Waals interactions. At very well-ordered, three 2D structures build up with specific interaction head-to-tail, head-on, tail-on, and sideways sequential order. This constitutes the first evidence that the van der Waals (vdW) intermolecular interactions between [7]thiaheterohelicene-2,13-carboxaldehyde molecules involved in the 2D assembly contribute to the formation of stable molecular structures on the surfaces. Furthermore, the theoretical calculations disclose quantitatively and clearly demonstrate why the 2D “MP” phase formed by [7]thiaheterohelicene2,13-carboxaldehyde on Au(111) terraces is more favorable than the “PP” (or “MM”) phase.

Keywords: Self-assembly, Au(111), 2D, van der Waals, ASED+, EHMO-ESQC, helicene.

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