PEOPLE'S DEMOCRATIC REPUBLIC OF ALGERIA
MINISTRY OF HIGHER EDUCATION AND SCIENTIFIC RESEARCH

UNIVERSITY OF MAY 8th, 1945 – GUELMA
FACULTY OF MATHEMATICS, COMPUTER SCIENCE
AND MATERIAL SCIENCES
LABORATORY OF APPLIED CHEMISTRY

4th (SNCA)

National Seminar

4ème SNCA 2025 Université de Guelma

on

Applied Chemistry

Book of Abstracts

27 November 2025

Foreword

It is with great honor and genuine pleasure that we present the proceedings of the **4th National Seminar on Applied Chemistry (SNCA'25)**, held on **November 27, 2025**, at the **University of May 8th, 1945 – Guelma**. This scientific event, organized by the **Laboratory of Applied Chemistry of the Faculty of Mathematics, Computer Science and Matter Sciences**, brought together researchers, academics, students, and professionals around the most current and innovative topics in applied chemistry.

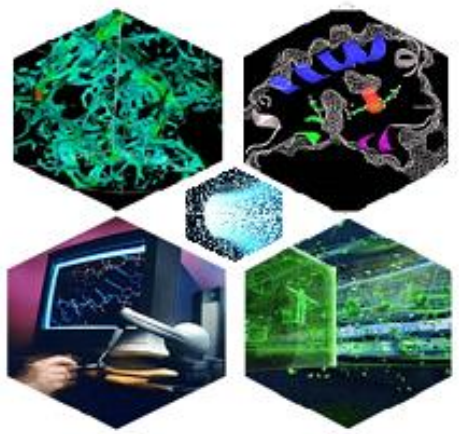
Applied chemistry, as a multidisciplinary field, plays a crucial role in the development of solutions to environmental, industrial, energy, and medical challenges. In this context, the seminar was enriched by high-level plenary lectures delivered by renowned experts, highlighting recent scientific advances and future perspectives in applied chemistry research.

This fourth edition of the seminar was structured around **four major scientific themes**, reflecting the diversity and richness of the presented works:

- ✓ **Theme 1:** Organic Synthesis, Medicinal Chemistry, Biochemistry, Pharmaceutical Chemistry, and Phytochemistry (Natural Products)
- ✓ **Theme 2:** Molecular Modeling and Theoretical Calculations
- ✓ **Theme 3:** Catalysis, Corrosion Chemistry, and Water Treatment
- ✓ **Theme 4:** Materials, Nanomaterials, Hybrid Materials, and Polymers

This book of abstracts reflects the quality and diversity of the scientific contributions presented during the seminar, including plenary lectures, oral communications, and poster presentations. These various forms of exchange fostered fruitful scientific discussions, contributing to knowledge sharing, strengthening collaborations, and promoting innovation in the field of applied chemistry.

We would like to express our sincere thanks to all participants, plenary speakers, contributors, as well as members of the organizing and scientific committees, for their commitment and valuable contributions to the success of this event. We hope that this book will serve as a source of inspiration and scientific reflection, and we wish you an enjoyable reading and fruitful scientific exchanges.



Message From the Chair

Dear Colleagues,

Following the successful completion of the **4th National Seminar on Applied Chemistry (SNCA'25)**, organized by the **Laboratory of Applied Chemistry** of the **Faculty of Mathematics, Computer Science and Matter Sciences, University of May 8th, 1945 – Guelma**, and held on **November 27, 2025**, it is with great honor and genuine pleasure that I express, on my own behalf and on behalf of all members of the Organizing Committee, our sincere gratitude to all participants and contributors for their commitment and valuable involvement.

We are proud to have brought together researchers, academics, and professionals around the most recent scientific advances, thus providing a constructive framework for dialogue, collaboration, and innovation. The themes addressed during the seminar clearly highlighted the central role of applied chemistry in the development of solutions to environmental, energy, industrial, and medical challenges.

This book of abstracts, which compiles high-quality scientific contributions, reflects the richness of the discussions and the significant advances presented throughout the event. We hope that this publication will serve as a valuable reference for participants, strengthen scientific collaboration, and inspire new perspectives and future research projects.

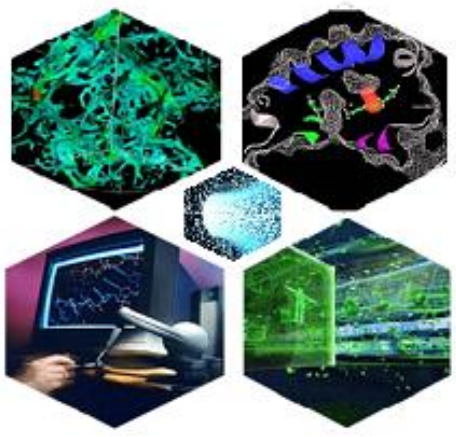
I would like to express my deepest appreciation to the **plenary speakers, Professor Mekki KADRI** from the **University of May 8th, 1945 – Guelma**, and **Professor Emeritus Nour-Eddine AOUF** from **BADJI Mokhtar University – Annaba**, for the excellence of their lectures and for the valuable scientific insight they brought to this edition of the seminar.

My sincere thanks also go to all speakers for the quality of their presentations, to the members of the **Scientific Committee** for their expertise and rigor, and to the **Organizing Committee** for their dedication and sustained efforts.

We hope that this seminar has met your expectations, both scientifically and personally, and that you will take away new ideas and stimulating perspectives for your future work. We look forward to welcoming you again at our forthcoming scientific events.

Yours sincerely,

Dr. Cheghib Nedjoua
Chair of the National Seminar on Applied Chemistry
Laboratory of Applied Chemistry
Faculty of Mathematics, Computer Science and Matter Sciences
University of May 8th, 1945 – Guelma



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Contacts:
Fax:037116471
Email:4.snca.2025@gmail.com

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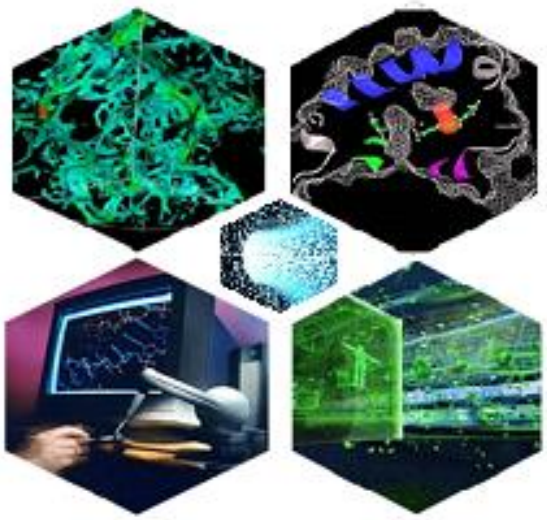
Table des matières

Plenary Conference



Les complexes de coordination et organométalliques : Approches expérimentale et par modélisation moléculaire, utilisations innovantes

Mekki KADRI, Professeur

Laboratoire de Chimie Physique, Université 08 Mai 45, BP40, Guelma 24000.
mekkadri@gmail.com

Résumé

L'interaction Ligand-ion métallique conduit à la formation d'un complexe de coordination comme le prévoit la théorie de Werner ou d'un complexe organométallique caractérisé par des liaisons ion métallique-carbone, selon la structure des réactifs et des conditions opératoires. Les espèces métalliques résultantes, trouvent de potentielles applications en catalyse, développement de nouveaux médicaments, de nouveaux matériaux, médecine, électronique, optique, magnétisme etc.
Durant la conférence seront présentés des orientations et des exemples d'études de la structure et des propriétés de ces associations, menées par voie expérimentale et par modélisation moléculaire. Par ailleurs, l'utilisation de ces complexes dans le développement de la plus innovante technique de traitement du cancer sera illustrée par la présentation de la thérapie photodynamique.

Mots clés : Complexes organométalliques, Ion métallique, Catalyse, Modélisation moléculaire, Approches expérimentales, Structure et propriétés, Thérapie photodynamique, Applications biomédicales.

Ecocatalysis and Asymmetric Organocatalysis, a New Vision of Green and Sustainable Chemistry

Nour-Eddine AOUF, Professeur Emérite

L.C.O.A. Groupe de Chimie Bio-Organique, Faculté des Sciences, UBM Annaba
aoufnoureddine18@gmail.com

Every year, we discover with horror that we are depleting the planet's resources faster and faster. Earth Overshoot Day marks the date when humanity's demand for ecological resources and services in a given year exceeds what Earth can regenerate in that year. In 2025, Earth Overshoot Day **lands on July 24**, the earth is now living on credit.

Green chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

Sustainable development as "development that meets the needs of the present without compromising the ability of future generations to meet their own needshe. 17 Sustainable Development Goals which are an urgent call for action by all countries it is a priority for the well- being of the planet.

Asymmetric organocatalysis has been a key part of pharmaceutical research and production. The methods pioneered by List and MacMillan have allowed synthesis of important molecules without the intensive use of environmentally damaging heavy metals.

A new vision of green and sustainable chemistry based on a well-established concept named Ecocatalysis, this strategy is based on the capacity of plants to adapt to stresses caused by high concentrations of metal elements in their environment;

In this contribution, we present some work from our group concerning the synthesis of α-aminophosphonates and hydroxyphosphonates, the chemistry of protective groups as well as the design of compounds for therapeutic purposes which use some principles of green chemistry.

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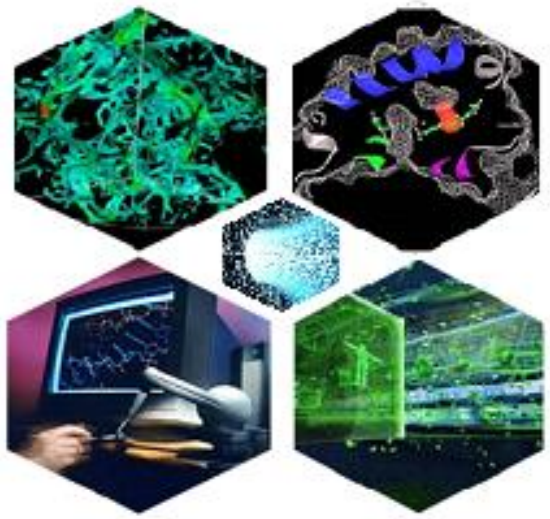
Theme 1:

Organic Synthesis, Medicinal Chemistry, Biochemistry, Pharmaceutical Chemistry, and Phytochemistry (Natural Products)



UPLC-ESI-MS/MS Profile and Biological Activities of Three Extracts from Various Zygophyllum Species

Abdeldjabbar Messaoudi[1]

[1] Department of Drilling and Mechanics of Oil Fields, Faculty of Hydrocarbons, Renewable Energies, Earth and Universal Sciences, University of Kasdi Merbah Ouargla, Algeria.
messaoudiabdeldjabbar@gmail.com

Abstract

Zygophyllum is a significant genus within the Zygophyllaceae family, prevalent in desert and arid locations, recognized for its anti-inflammatory, antioxidant, antibacterial, and anticancer attributes. three main species of the genus Zygophyllum. Phenolic components of Zygophyllum species (Z. album, Z. cornutum, and Z. gaetulum) from southern Algeria were studied using UPLC/MS-MS. Nineteen phenolic compounds were discovered, with Esculin Hydrate, Catechin, and Thymol as the principal ingredients. The cytotoxicity testing of three Zygophyllum ethanolic extracts on Saccharomyces cerevisiae indicated that both Z_{Al} and Z_{Co} extracts are non-toxic at all evaluated doses. The Z_{Ga} extract markedly reduced cell viability by approximately 50% at the maximum dose of 10,000 µg/ml. The anti-inflammatory efficacy of Zygophyllum extracts exhibited considerable variation across distinct doses. Aspirin, utilized as a benchmark, exhibited a dose-dependent impact, with a maximum inhibition of 72.7% at a concentration of 20 mg/ml. At the identical concentration, Z_{Ga} demonstrated the most pronounced effect at 50.8%, succeeded by Z_{Co} at 27.2%. and Z_{Al} at 17.7 percent. The IC50 values obtained from the Alpha-amylase assay revealed notable disparities in the potency of the evaluated substances. Z_{Al} exhibited the greatest potency with an IC50 of 3.7, signifying efficacy but necessitating a higher dose than Acarbose.

Keywords: Zygophyllum, ethanolic, cytotoxicity, anti-inflammatory, alpha-amylase.

Extraction et caractérisation des polysaccharides issus des noyaux de dattes : application à la synthèse de nanoparticules à activité antioxydante

Amina DOGHMANE[1*], Zahara RAZKALLAH[1], Sana ABDELLIOUI[1], Rouba RAHEM[2], Chaima KIRATI[2]

[1] Laboratory of Biology, Water and Environment, Department of Biology, University of 8 May 1945 Guelma, Algeria
[2] Department of Biology, University of 8 May 1945 Guelma, Algeria

Résumé :

Les noyaux de dattes représentent un sous-produit agroalimentaire encore peu exploité, bien qu'ils soient riches en composés bioactifs tels que les polysaccharides. Dans cette étude, nous avons visé la valorisation de ces résidus par l'extraction des polysaccharides hydrosolubles et l'évaluation de leur potentiel dans la synthèse de nanoparticules à activité antioxydante. Les polysaccharides ont été extraits à partir de noyaux de dattes broyés à l'aide d'une extraction aqueuse suivie d'une précipitation à l'éthanol. Les extraits obtenus ont ensuite été caractérisés par le dosage des sucres totaux (méthode du phénol-sulfurique) et des protéines (méthode de Bradford). Par la suite, ces polysaccharides ont été utilisés comme agents réducteurs et stabilisants pour la synthèse de nanoparticules d'argent AgNPs, réalisée selon une méthode verte sans recours à des solvants toxiques, leur synthèse a été confirmé par un balayage spectrophotoscopique dans l'intervalle de 200-500 nm. Les résultats ont montré que les extraits polysaccharidiques contenaient une proportion importante de sucres totaux et une faible teneur en protéines, confirmant leur pureté. Les nanoparticules obtenues sont caractérisées le changement de couleur et par spectrophotométrie avec un pic d'absorbance à 430nm qui représente le phénomène a résonance plasmonique de surface qui caractérise les NPs. Leur activité antioxydante, évaluée par le test DPPH, a révélé une capacité de piégeage des radicaux libres significative, dépendante de la concentration. En conclusion, les polysaccharides extraits des noyaux de dattes se sont avérés être des biomatériaux prometteurs pour la synthèse de nanoparticules antioxydantes, ouvrant la voie à une valorisation durable des sous-produits de dattes dans les domaines pharmaceutique et agroalimentaire.

Mots clés : Polysaccharides, Noyaux de dattes, AgNPs, Activité antioxydante

A Review on Phytotherapy for Obesity: The Role of Bioactive Compounds

Ouisseme BELGHIT[1], Khedidja AMIRA[1, 2], Hicham BOUGHENDJIOUA[1, 2]

[1]Department of Natural Sciences, Higher Normal School of Technological Education of Skikda, Skikda, Algeria.
[2]Laboratory of Physical, Chemistry and Biology of Materials, Skikda, Algeria.
Corresponding author: Ouisseme BELGHIT (belghit.ouissem@enset-skikda.dz)

Abstract

Obesity is a growing global health concern influenced by a combination of genetic, environmental, hormonal, and lifestyle factors. Because of the side effects and limitations of conventional medications, medicinal plants have been increasingly investigated as safer and more sustainable alternatives. Their rich content of bioactive compounds, has demonstrated potential in regulating metabolic pathways involved in obesity management.

Recent studies have reported that medicinal plants such as red raspberry, Garcinia, henna, red grape, soybeans, green tea, Moringa, and olive exhibit significant anti-obesity activity. These plants contribute to weight reduction, lower total cholesterol and triglyceride levels, and raise HDL cholesterol. Additionally, they enhance lipase activity, inhibit visceral fat synthesis, and reduce blood glucose levels. Their beneficial effects are attributed to flavonoids, tannins, and phenolic acids, which possess potent antioxidant, anti-inflammatory, and lipid-regulating properties that counteract oxidative stress—a key factor in obesity-related metabolic disorders.

Overall, these findings highlight the promising potential of medicinal plants as safer, cost-effective, and holistic strategies for long-term obesity management and the prevention of metabolic disorders.

Keywords: Obesity, medicinal plants, bioactive compounds, oxidative stress, plant-derived medications.

Potentiel bioactif des huiles essentielles algériennes : une approche intégrée des activités antioxydantes et antibactériennes

Abdelkader Oumeddour[1], Benhalima Lamia[2]

1 Département des sciences de la nature et de la vie, Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre et de l'Univers, Université 08 Mai 1945, Guelma 24000, Algérie
2 Département de biologie, Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre et de l'Univers, Université 08 Mai 1945, Guelma 24000, Algérie.

Abstract

Cette étude met en évidence la diversité chimique et biologique des huiles essentielles (HE) algériennes à travers l'évaluation comparative de leurs activités antioxydantes et antibactériennes. L'analyse de 70 espèces issues de 25 familles révèle une large variabilité d'activité. Les tests DPPH montrent des valeurs d'IC_{50} comprises entre 8,4 et 195 µg/mL, avec une forte activité chez Daucus muricatus (8,4 µg/mL), Artemisia campestris (9,6 µg/mL), Thymus ciliatus (12,3 µg/mL) et Pimpinella anisum (13,7 µg/mL), dominées par des terpènes oxygénés tels que carvacrol, thymol, camphre, 1,8-cinéole et α-thuyone. Sur le plan antibactérien, les zones d'inhibition varient de 12 à 36 mm, les HE de Thymus vulgaris (36 mm), Rosmarinus officinalis (33 mm), Eucalyptus globulus (31 mm) et Citrus aurantium (30 mm) se montrant les plus actives. Ces effets sont liés à la synergie des phénols et alcools monoterpéniques perturbant la membrane bactérienne. Les espèces T. ciliatus, A. campestris et R. officinalis se distinguent par une double activité antioxydante et antibactérienne marquée. Ces résultats confirment le rôle clé des composés oxygénés et positionnent la flore aromatique algérienne comme une source prometteuse de molécules bioactives à fort potentiel pharmaceutique et agroalimentaire.

Keywords : Huiles essentielles algériennes, Activité antioxydante, Activité antibactérienne, Composés bioactifs.

Séparation, Identification Et Activité Antioxydante D'un Flavonoide Isolé D'une Espèce Du Genre Centaurea

Meroua AHMED CHAOUCH [1], Thamere CHERIET [1], Ramdane SEGHIRI [1], Ratiba MEKKIOU [1], Ouahiba BOUMAZA [1]

[1]Unité de valorisation de ressources naturelles, molécules bioactives et analyse physicochimique s et biologiques (VARENBIOMOL), Université des frères Mentouri Constantine 1, Faculté des Sciences, Route Ain El Bey 25000 Constantine, Algeria.
Corresponding author: AHMED CHAOUCH Meroua (Ahmedchaouch0111@gmail.com)

Abstract

L'investigation phytochimique des plantes médicinales représente actuellement un potentiel inestimable pour la découverte de nouvelles substances chimiques bioactives, dans ce contexte et vu l'importance et la richesse des plantes en métabolismes secondaires notre choix s'est porté sur le genre Centaurea. La recherche bibliographique ethno médicale a montré que les espèces de ce genre sont très utilisées en médecine traditionnelle notamment en Algérie pour leur richesse. Le protocole d'extraction a débuté par une macération dans un système hydro-méthanolique ($MeOH/H_2O$; 80 :20 ; v/v) suivi par des extractions liquide-liquide par des solvants de polarité croissante : chloroforme, acétate d'éthyle et n-butanol. L'étude phytochimique de l'extrait acétate d'éthyle a permis l'isolement d'un squelette flavonique à l'état pur dont la détermination structurale a été faite sur la base des données du spectre RMN ^1H et des données spectroscopiques UV-Visible. Le dosage de l'activité anti-oxydante a été effectué sur cette molécule pour identifier son pouvoir anti oxydant.

Keywords : extraction, Centaurea, pouvoir antioxydant, squelette flavonique, polyphénol

Inclusion Complex Formation of β-Cyclodextrin with a New Brominated Bis-8-Hydroxyquinoline Derivative (β-CD-3q): Spectroscopic and Physicochemical Investigation

Nedjoua CHEGHIB*[1], Wafa SOUDANI [2], Samia BENRABAH[3], Rafik MAIZI[1], Abdel-Ghani BOUDJAHEM[1], Meryem DERDARE[1], Yasmine MEZARI[1], Bochra BENCHEIKH[1], Salma Amrani[4], Elhadj KOLLI[5]

[1] Computational and Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, P.O. Box 401, Guelma 24000, Algeria.
[2] Department of Pharmacy, Laboratory of Organic Chemistry, Badji-Mokhtar Annaba University, Annaba, Algeria.
[3]Department of Geology, Geology Research Laboratory (GRL), Faculty of Earth Sciences, Badji Mokhtar – Annaba University, P.O. Box 12, 23000, Annaba, Algeria
[4] Faculté FMISM, University 08 mai 45Guelma, Algeria
[5]Laboratory of Silicates, Polymers and Nanocomposites, Faculty of Science and Technology, University 8 May 1945 – Guelma 24000, Algeria.
Corresponding author: nedjoua11_c@yahoo.fr

Abstract:

The development of pharmaceutical formulations based on cyclodextrin (CD) inclusion complexes with bis-8-hydroxyquinoline derivatives (HQNBA) represents a promising strategy for improving solubility, stability, and biological performance. In this context, the present study focuses on the pharmacomodulation of a new molecule, 5,5'-(((2-bromophenyl) azanediyl) bis (methylene)) bis(quinolin-8-ol), and its ability to form an inclusion complex with β-cyclodextrin (β-CD). The β-CD–3q inclusion complexes were prepared both in solution and by co-precipitation. Inclusion capability and complex stoichiometry were evaluated using UV-visible spectroscopy. Physicochemical and spectral analyses in the solid state (IR, UV-visible, Rf, Pf) enabled the structural elucidation of the isolated products and confirmed the successful formation of the β-CD–3q inclusion complex.

These findings highlight the potential of brominated HQNBA derivatives for the development of cyclodextrin-based formulations with promising pharmaceutical applications.

Keywords: β-cyclodextrin, inclusion complex, bis-8-hydroxyquinoline, brominated derivative, UV-visible spectroscopy, pharmacomodulation.

Conversion of Sulfamido-phosphonate to Sulfamate-phosphonate under Nitrosation Conditions and Evaluation of Their Antiproliferative Activity

Zineb Aouf [1], Houria Bentoumi [1], Rachida Mansouri[2], Abdeslam Bouzina[1], Nour-Eddine Aouf[1]

[1] Laboratory of Applied Organic Chemistry, Bioorganic Chemistry Group, Sciences Faculty, Chemistry Department, Badji Mokhtar-Annaba University, Box 12, 23000 Annaba, Algeria.
[2] Environmental Research Center (CRE), Alzone 23000, BP 72 A Menadia Annaba, Algeria.[3]Department, Laboratory, University, City, Country
Corresponding author: AOUF Zineb (zineb.aouf@univ-annaba.dz)

Abstract

Sulfamate derivatives constitute a versatile and pharmacologically important family of organo-sulfur compounds characterized by the presence of the sulfamoyl functional group (RO-SO_2-NH-R'). This moiety is known to impart unique physicochemical properties and broad biological activities, including anticancer, antiglaucoma and enzyme inhibitory effects.[1] In particular, several sulfamate-based drugs, such as Topiramate and estrone sulfamate (EMATE), have demonstrated potent anticonvulsants and steroid sulfatase inhibitory properties, highlighting the therapeutic relevance of this class.[2] Owing to their structural flexibility, sulfamate derivatives can be easily modified or incorporated into hybrid systems to enhance biological performance. [3]
In the present study, we describe the rearrangement of sulfamidophosphonates (prepared through a Kabachnik-Fields one-pot reaction) into sulfamate-phosphonates under nitrosation conditions using $NaNO_2$ and formic acid (HCOOH). The resulting sulfamatephosphonate derivatives were thoroughly characterized by spectroscopic techniques, including IR, NMR, and MS.
The antiproliferative activity of the synthesized sulfamate-phosphonate derivatives was evaluated **in vitro** against a panel of human cancer cell lines, including Huh7 (hepatocellular carcinoma), D12 (breast cancer), $CaCo_2$ (colorectal adenocarcinoma), MDA (breast adenocarcinoma), HCT 116 (colon carcinoma), PC3 (prostate carcinoma), NCI–H727 (lung carcinoma), and MCF7 (breast carcinoma). Each compound was tested at a concentration of 25 µM for 48 hours, using DMSO as a negative control and doxorubicin and taxol as positive controls. **The obtained results demonstrated encouraging antiproliferative profiles, highlighting the potential of sulfamatephosphonate scaffolds as promising candidates for further development of novel anticancer agents.**

Keywords: Sulfamate-phosphonates, Sulfamidophosphonates, Nitrosation conditions, Antiproliferative activity

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Potentiel Antioxydant Et Richesse Phytochimique D'une Plante Medicinale Et Aromatique Algerienne

Soraya BELAID [1]□, Salah Eddine DJILANI [2], Amani ZIANI [3]

[1]Materials Physico-chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid El Tarf University, P.B. 73, El Tarf 36000, Algeria
[2]Laboratory of Synthesis and Organic Bio catalysis (LSBO), Department of Chemistry, Badji Mokhtar-Annaba University, Box 12, Annaba 23000, Algeria.
[3]Department of Chemistry University of Chadli Bendjedid - El Tarf BP 73 El Tarf 36000 Algeria

s.belaid@univ-eltarf.dz

Résumé:

La Mentha spicata L. (menthe verte) est une plante médicinale couramment employée en Algérie, aussi bien en cuisine comme plante aromatique, mais également en médecine traditionnelle pour ses propriétés digestives, antiseptiques et rafraichissantes. Elle fait partie de la famille des Lamiaceae et se caractérise par sa teneur élevée en composés phénoliques et flavonoïdes, qui sont à l'origine de ses multiples propriétés biologiques. Des recherches ont démontré une activité antioxydante importante, due à la présence des composés tels que le menthol, le menthone, l'acide rosmarinique et la lutéoline. Ces composés permettent de neutraliser les radicaux libres, réduisant le stress oxydatif et prévenant certaines pathologies dégénératives. Par conséquent, la menthe verte est une ressource naturelle importante en antioxydants, abondamment présente dans la flore algérienne.

Mots clés : plante médicinale, Mentha spicata, activité antioxydante, test DPPH, Huiles essentielles.

Phytochemical Analysis and Biological Activity of An Algerian Saharan Plant of Poaceae Family

Nourelhouda BENELMUFTI[1*], Hamza FADEL[1], Sabrina BICHA[1], Nabila SLOUGUI11[2], Thamere CHERIET[1,3], Hichem HAZMOUNE[1] et Ouahiba BOUMAZA[1]

[1]Research Unit, Valorization of Natural Resources, Bioactive Molecules and Physicochemical and Biological Analyzes (VARENBIOMOL), University of Mentouri Brothers Constantine 1, Ain El-Bey Road, 25000, Constantine, Algeria.
[2]National Polytechnic School of Constantine.
[3]Département de science de la matière, Faculté des sciences exactes et sciences de la nature et de la vie, Université Larbi Ben M'hidi-Oum El-Bouaghi, Algeria

E-mail : benelmuftinorelhouda@gmail.com

Abstract

The choice of quantifying the polyphenols is due to their very interesting biological activities, the same applies to flavonoids. The specific objectives were to investigate phytochemical profile using HPLC-DAD of aerial parts extracts from an Algerian Saharan plant of Poaceae family with its evaluation of the total phenol and flavonoid content Dried aerial parts of our species (1700 g) were macerated in a hydro-alcoholic mixture (Methanol: Water, 80:20, v: v). Therefore, the obtained methanolic crude extract was subjected to liquid-liquid extraction using solvents of increasing polarity to get chloroform, ethyl acetate and n-butanol extracts, respectively. Moreover the extracts were evaluated to analyze the chemical profile using HPLC-DAD and to determine the total phenol and flavonoids contents using Folin-Ciocalteu and Aluminium trichloride methods respectively. The HPLC-DAD profile revealed the presence of 17 compounds, with epicatechin (78.06 mg/g), gallic acid (32.20 mg/g), rutin (22.18 mg/g), luteoline-7-glucoside (9.09 mg/g) and caffeic acid (8.51 mg/g) being the main ingredients. While for quantitative analysis the results showed that AcOEt extract was the most concentrated in polyphenols than $CHCl_3$ and n-BuOH extracts (129, 48; 112,44 and 42,24 µgGAE/mg, respectively), and for the flavonoids the n-BuOH extract has the higher value compared to AcOEt and $CHCl_3$ extract (56.44; 33.71 and 6.34 µgQE/mg, respectively), with moderate antioxidant capability (IC50 = 2.89 ± 0.11 µg/ml).

Mots clés: Poacea, HPLC-DAD, total phenol content and flavonoid content.

Synthesis And Characterization of Novel Imidazoles Derivatives with Guanyl Hydrazone Moiety

Ghadir BOUKERTOUTA [1], Achour SERIDI [1].

[1]Department of Matter Science, Physical Chemistry Laboratory, 8 May 1945 University, Guelma, Algeria.
Corresponding author: BOUKERTOUTA Ghadir (boukertouta.ghadir@univ-guelma.dz).

Abstract

Heterocycles such as imidazoles and triazoles are considered very crucial scaffolds in the discovery and development of biologically active agents (drugs). Guanylhydrazone moiety is one of the most widely used scaffolds in the design and development of novel lead compounds for their numerous activities as an anticancer, antibacterial and antifungal agent.
In this Poster, imidazoles derivatives were synthesized from condensation reaction between isatin and various substituted guanylhydrazones yielded imidazole derivatives.
The synthesized compounds were characterized using various spectral techniques such as ^{1}H NMR, ^{13}C NMR and IR.
^{1}H-NMR spectra of these imidazole derivates showed a singlet in the downfield region around 12.46-12.04 ppm and 8.02-8.42 ppm corresponding to the imidazole nitrogen to hydrogen and CH=N. The IR spectrum of the target compounds all demonstrated the N-H stretching bands around 3409 and 3347 cm^{-1} and the imine (C=N) bands at 1647 to 1607 cm^{-1}.

Keywords: Imidazole, Guanylhyrazone, Reflux sunthesis, NMR, IR.

Synthesis, Characterization and Antibacterial Properties of 2-Aminophenol-Based Compound

Naouel Boudraa[1], Ouafa Boukhemis[1,2], Abdelkader Mahrouk[1,3], Rachida Assabaa[4]

[1]Biotechnology Research Center- CRBt Constantine, Algeria
[2]Research Unit for Environmental Chemistry and Structural Molecular Chemistry (CHEMS), Department of Chemistry, Constantine 1- Frères Mentouti University, Constantine, Algeria.
[3]Laboratory of Applied Biochemistry, Faculty of Natural and Life Sciences, Constantine 1- Frères Mentouti University, Constantine, Algeria.
[4]Department of Chemistry, Constantine 1- Frères Mentouti University, Constantine, Algeria.
Corresponding author: Naouel Boudraa (bnaouel@gmail.com)

Abstract

An aminophenol derivative was synthesized and thoroughly characterized using spectroscopic techniques, including infrared (IR) and UV-Visible spectroscopy. Its molecular structure was determined by single-crystal X-ray analysis, which revealed that the synthesized imine exists in a zwitterionic form with an almost planar geometry. The compound was evaluated for its antibacterial properties against five bacterial strains, including three Gram-negative bacteria — Escherichia coli ATCC 8739, Salmonella typhi ATCC 14028, and Pseudomonas aeruginosa ATCC 9027 — and two Gram-positive bacteria — Bacillus subtilis subsp. spizizenii ATCC 6633 and Staphylococcus aureus ATCC 6538. The results showed significant antibacterial activity against all tested strains.

Keywords: Aminophenol, Imine, Single-Crystal X-Ray Diffraction, Synthesis, Antimicrobial activity.

Phytochemical Study of the Ethanolic Extract of Rosmarinus officinalis from the Guelma Region

Hanane Nadia Boussenane [1,2*], Boukamara Hanane[1], Kaidi Souad[1], Mairif Samah[1] Bouden Ismail[1], Endjeddou Dalila[1]

[1,] Laboratoire de Biologie Moléculaire et Cellulaire
Université 8 Mai 1945 Guelma, Algérie.
Auteur Correspondant e-mail : nboussenane@yahoo.com

ABSTRACT

Rosmarinus officinalis is a medicinal and aromatic plant containing several secondary metabolites such as flavonoids, terpenoids and polyphenols. The objective of our work is to highlight the medicinal plant of Rosmarinus officinalis from the region of Guelma in Algeria by the quantification of the contents of phenolic compounds and flavonoids.
This plant was subjected to a phytochemical screening to highlight the qualitative composition of the plant in secondary metabolites. This analysis shows the presence of alkaloids, flavonoids, saponins, tannins, mucilages, sugars and polysaccharide reducing compounds.
The extraction of the raw extract was made by hydro-ethanolic maceration at 70%. The yield is around 7.84%. Subsequently, we performed thin layer chromatography (TLC) with two different solvent systems. The first system consists of solvents (hexane / ethyl acetate / ethanol / n-butanol / chloroform) 2:8:1.5:3:20 by volume and the second system consists of solvents (ethan / H2O) 7:3 by volume. By the help of this TLC, we were able to observe several distinct colors representing different secondary metabolites.
The dosage of total polyphenols by the method of Folin coicalteu showed that the hydro-ethanolic extract of Rosmarinus officinalis is very rich in phenolic compounds.
The determination of total flavonoids by the aluminum trichloride method also showed the hydro-ethanolic extract of rosemary is very rich in flavonoid compounds.
The determination of the antiradical activity (radical DPPH) using ascorbic acid as a standard show that the hydro-ethanolic extract of rosemary has significant antioxidant power. The values of the 50% inhibitory concentrations were determined graphically; they are equal to 223 µg/ml and 75 µg/ml for the hydro-ethanolic extract and the ascorbic acid respectively.

Keywords: Rosmarinus officinalis, secondary metabolites, phenolic compounds, flavonoids, alkaloids.

New N-(substituted) Sulfonyl Carboxamides bearing Pyrrolidine-2, 5-dione: Synthesis and Computational Analyses

Chafika BOUGHELOUM [*1], **Soumaya BOUSKIA** [1]

[1] Laboratory of Advanced Systems and Materials, Sciences Faculty, Badji Mokhtar-Annaba University, P.o. Box 12, Annaba. 23000, Algeria.

*E-mail : chafika.bougheloum@univ-annaba.dz
c.bougheloum@gmail.com

Abstract

Pyrrolidine-2,5-diones, or succinimides, are intriguing heterocyclic compounds because of their pharmacophoric status and fundamental biological properties.
These compounds have demonstrated promising efficacy in treating a number of diseases, such as cancer, inflammation, epilepsy, and microbial infections.
Furthermore, sulfonamide derivatives have been used pharmacologically to treat some illnesses. These drugs' low cost, minimal toxicity and remarkable therapeutic potential make them popular for treating and preventing a wide range of infections in humans.
The combination of two bioactive components results in a new molecule that may be used as a lead compound in drug discovery efforts.
For this reason, a simple synthesis of pyrrolidine-2,5-dione with a sulfonamide moiety was reported in this study.
Molecular docking simulation was used to investigate the reactivity of the synthesized compounds and their potential binding mode to the active site of the tyrosyl-tRNA synthetase protein (PDB ID: 1JIJ). The absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction of the synthesized molecules was also examined.

Keywords: Pyrrolidine-2,5-dione, Carboxamide, Sulfonamide, Molecular docking, ADMET.

Combined theoretical and experimental study of new vanillin-based derivatives: Structural insights, unusual reactivity, and biological applications

Chaima Aouachria[a], Haoua Hamana[a], Lakhmissi Kaboub[a], and Abdelkrim Gouasmia[a].

[a] Laboratory of Organic Materials and Heterochemistry, University of Tebessa, Tebessa, 12000, Algeria,
E-mail addresses: chaima.aouachria@univ-tebessa.dz

Abstract

The remarkable chemical versatility of vanillin makes it a valuable scaffold for the functionalization of aromatic systems, offering promising prospects in materials science and pharmaceutical applications. In this study, we uncover an unconventional reactivity pattern occurring at an unusually reactive site of vanillin's aromatic ring, governed by the electronic influence of its hydroxyl and methoxy substituents. Within this framework, we report the synthesis of two unprecedented vanillin-derived compounds: 3-(5,6-dihydro-[1,3]dithiolo[4,5-b][1,4]dithiin-2-yl)-4-hydroxy-5-methoxybenzaldehyde (I) and 3-(4,5-bis(methylthio)-1,3-dithiol-2-yl)-4-hydroxy-5-methoxybenzaldehyde (II), obtained through reactions of vanillin with 4,5-ethylenedithio-1,3-dithiole-2-thione (A) and 4,5-bis(methylthio)-1,3-dithiole-2-thione (B), respectively.

Computational investigations based on density functional theory (DFT) were employed to rationalize this unexpected substitution pathway, providing mechanistic insights consistent with the experimental observations. Structural elucidation using single-crystal X-ray diffraction, complemented by Hirshfeld surface analyses, revealed the presence of notable non-covalent interactions such as sulfur–sulfur (S···S) contacts and hydrogen bonds, which play a key role in stabilizing the supramolecular organization of these molecules.

Preliminary biological evaluations indicated that both compounds exhibit significant antimicrobial, antioxidant, and anti-inflammatory activities, emphasizing their potential as bioactive frameworks. The unique combination of structural originality and biological effectiveness positions these vanillin derivatives as promising candidates for future development in therapeutic and functional material applications. Overall, this work broadens the chemical landscape of vanillin and provides new insights into its untapped reactivity and material relevance.

Keywords: Vanillin derivatives, Structural analysis, Theoretical studies, Unconventional reactivity, Hydrogen bonding, biological activity.

Synthesis and Theoretical Evaluation of a New α-aminophosphonate Derivative

Djamila Roua AISSAOUI[1], Abdelkader HELLAL[1], Yacine NOUAR[1]

[1]Laboratory of Electrochemistry of Molecular Materials and Complexes (LEMMC). Department of Process Engineering, Faculty of Technology, Sétif 1-Fertat ABBAS University.
aissaoui.d.r00@gmail.com

Abstract
Combining computational approaches with experimental synthesis is a powerful strategy for identifying promising bioactive molecules. α-aminophosphonate, in particular have attracted attention due to their structural diversity and potential biological activities. This work aimed to synthesize a novel α-aminophosphonate derivative via the Kabachnik–Fields reaction and evaluate its electronic propreties using Density Functional Theory (DFT) calculations. Molecular docking studies using autodock vina were performed to predict the binding mode and the affinities of the compound toward a selected protein target while ADME analyses evaluated pharmacokinetic behavior and drug-likeness. The findings indicate that the synthesized compound shows favorable electronic, binding, and pharmacokinetic features, supporting its advancement to biological assays and structure-activity relationship studies.

Keywords: Synthesis, electronic properties, molecular docking, pharmacokinetic.

Caractérisation préliminaire des métabolites secondaires présents dans les feuilles de Pelargonium graveolens

Nour El-Houda Djeghader[1,2], Khedidja Amira [2,3], Meriem Snani[3,4]

[1]Departement de Biologie, Faculté des Sciences, Université BADJI Mokhtar- Annaba, Algérie.
[2]Laboratoire de Physique, Chimie et Biologie des matériaux, ENSET- Skikda, Algérie.
[3] Département des Sciences naturelles, Ecole Normale Supérieure de l'Enseignement Technologique- Skikda, Algérie

[4]Laboratoire de Recherche d'Ecophysiologie Animale, Université BADJI Mokhtar- Annaba, Algérie.

Corresponding author: Nour El-Houda DJEGHADER (djeghader_nour@yahoo.fr)

Résumé

Pelargonium graveolens, est une plante aromatique largement utilisée en cosmétique et en médecine traditionnelle pour ses propriétés antimicrobiennes, antioxydantes et anti-inflammatoires. Sa richesse en composés volatils et phénoliques en fait une source prometteuse de molécules bioactives d'intérêt pour la phytothérapie.
Les feuilles de Pelargonium graveolens ont été récoltées en avril 2025 dans la région de Sidi Harb (Annaba, nord-est de l'Algérie) pour une étude phytochimique préliminaire. L'objectif de ce travail est de détecter qualitativement les principales familles de métabolites secondaires à l'aide de tests colorimétriques simples.
L'extrait aqueux obtenu a été soumis à plusieurs réactions classiques. Les tests ont révélé la présence de flavonoïdes (réaction positive avec l'hydroxyde d'ammonium), de tanins (coloration noire avec le chlorure ferrique), d'alcaloïdes (coloration brun-rougeâtre avec le réactif de Wagner), de saponines (formation persistante de mousse après agitation) et de terpènoïdes. Ces résultats confirment la richesse de cette espèce cultivée localement en composés bioactifs, pouvant justifier certaines de ses activités biologiques traditionnelles rapportées dans la littérature.

Mots clés : Pelargonium graveolens, métabolites secondaires, feuilles, étude phytochimique.

Étude comparative de l'activité antibactérienne des extraits de Carthamus Carduncellus L.

Elhadj KOLLI[1], Samir ZEROUAL[2], Yassine AIMENE[3], Nedjoua CHEGHIB[4]

[1]Laboratoire des silicates, polymères et des nanocomposites, Faculté des Sciences et de la Technologie, Université 08 Mai 1945 Guelma 24000, Algérie.
[2]Laboratory of Genetics, Biotechnology and Valorization of Bio-resources, Faculty of Exact Sciences and Nature Sciences and the Life, University Mohamed Khider, Biskra, Algeria
[3]Laboratoire de chimie physique, Faculté des Mathématiques et de l'Informatique et des Sciences de la Matière, Université 08 Mai 1945 Guelma 24000, Algérie.
[4]Laboratoire de chimie Appliquée, Faculté des Mathématiques et de l'Informatique et des Sciences de la Matière, Université 08 Mai 1945 Guelma 24000, Algérie.

E-mail : kolli.elhadj@univ-guelma.dz

Résumé

L'utilisation des plantes pour traiter certaines affections remonte à l'Antiquité. Les Égyptiens et les Grecs utilisaient l'aloe vera pour soigner les irritations cutanées, les brûlures et les plaies. Aujourd'hui, de nombreux remèdes à base de plantes sont utilisés en médecine moderne, comme la digoxine, un médicament extrait de la digitale, utilisé pour traiter certains cas d'insuffisance cardiaque. Carthamus carduncellus L. est une espèce végétale appartenant à la famille des Astéracées. C'est une petite plante herbacée vivace aux feuilles basales, en forme de rosette, divisées en lobes terminés par des épines. La corolle est tubulaire, bleue ou violette. Peu de travaux ont été réalisés sur cette plante concernant la composition chimique de ses huiles essentielles, ses extraits ainsi que leurs activités biologiques. Pour ces raisons, nous avons préparés différents extraits dans le but d'évaluer leurs activités antibactériennes et de réaliser une étude comparative. La méthode utilisée dans cette activité est de diffusion sur disque en milieu gélosé Mueller-Hinton. Trois extraits ont été préparés : un extrait de Soxhlet éthanol 75 %, un autre par décoction et le troisième par un mélange EtOH / EtOAc (50 : 50, v/v). Les souches bactériennes employées dans cette étude sont Staphylococcus aureus ATCC 29213, Escherichia coli ATCC 25422, Pseudomonas aeruginosa ATCC 27953 et Staphylococcus aureus.

L'extrait d'EtOH/ EtOAc a montré une activité limitée, observée uniquement à doses élevées sur S. aureus (clinique) et P. aeruginosa, et sans effet sur E. coli. Alors que les deux autres extraits ne présentent aucun effet inhibiteur notable, suggérant leur inefficacité dans les conditions expérimentales.

Mots clés : Carthamus carduncellus L, Activité antibactérienne, Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa.

Évaluation de l'activité antibactérienne de l'huile essentielle "Thymus vulgaris vis-à- vis de souches d'Escherichia coli isolées à l'hôpital Ibn Zohr de Guelma

Farah ABID (1), Mabrouka BOUACHA (2), Nafissa BOUTEFNOUCHET (3)

[1]Laboratoire de Biologie moléculaire, département de Biologie, faculté de de nature et de la vie et sciences de la terre et de l'univers, université 8 mai 1945.

[2]laboratoire de toxicologie environnementale

[3] Laboratoires de microbiologie biochimie, département de Biochimie, faculté de science, université Baji mokhtar. Annaba.

farahabid72@gmail.com.

Les souches de Escherichia coli sont parmi les bactéries multirésistantes qui doivent être suivies constamment par les services d'hygiènes à l'hôpital, car en raison de ses résistances aux antibiotiques peuvent induire à des échecs thérapeutiques. L'aromathérapie figure parmi les outils dont disposent les aromathérapeutes, aromatologues et les naturopathes. Elle est très utile contre certaines affections. Son action la plus probante est de nature antibactérienne. On s'en sert donc très efficacement pour l'hygiène des espaces intérieurs à la maison, en soins esthétiques et pour la détente, et de plus en plus fréquemment en prévention et traitement des maladies infectieuses nosocomiales dans les milieux hospitaliers.

l'objectif de notre recherche est de de tester l'activité antibactérienne de l' huile essentielle"Thymus vulgaris" extraite de la plante aromatique le thym, sur une des espèces du genre Escherichia qui est Escherichia coli, cette bactérie a émergé comme l'un des agents pathogènes humains les plus importants, et a été au cours des dernières décennies, une des principales causes des infections hospitalières et communautaires, en raison de l' acquisition de résistance vis-à-vis des antibiotiques usuellement prescrits. Cette recherche laisse entrevoir une voie de recherche dans la lutte contre les souches d'Escherichia coli multirésistantes aux antibiotiques et tente de trouver un véritable espoir d'alternative thérapeutique en utilisant l'aromathérapie.

Ainsi des souches d'Escherichia coli ont été isolés à partir de produits pathologiques de patients admis à l'hopitall Ibn Zohr de Guelma et ont été testés avec des extraits de "thymus vulgaris" dont l'efficacité a été mise en évidence grâce la détermination de leurs CMI et CMB.

Mots clés : Thymus vulgaris - CMB - activité antibactérienne- Aromathérapie.

Charge Transfer Complexes Between Resveratrol And π- Acceptors; Parametric Study and Spectroscopic Characterisation

Fatima Zahra Hamamdia[1], Hanene Messiad[2] and Habiba Guebailia[3]

[1, 3] Department of Material Sciences, Faculty of Mathematics, Computer Science and Material Sciences, University of May 8, 1945 Guelma, 24000, Guelma, Algeria.
[2] Department of Environmental Process Engineering, ST Faculty, University of Constantine 3, 25056, Algeria.
Corresponding author: Fatima Zahra Hamamdia (fatimachimie82@gmail.com)

Abstract

Resveratrol is one of the most crucial active ingredients of plant origin from the stelbenoid family, found in grapes, berries, and peanuts that offers benefits including antioxidant, anti-inflammatory, and heart-protective effects. It may help protect against chronic diseases like cardiovascular disease, cancer, and Alzheimer's by reducing oxidative stress and inflammation.
However, the low bioavailability of this molecule, similar to that of the majority of polyphenols after their oral administration, hinders their exploitation as drugs. In order to circumvent this limitation, the inclusion of these compounds in cyclodextrins, as well as their complexation by charge transfer, is emerging as a potential strategy to optimize their biological properties.
This study aims to examine the interaction of resveratrol with DDQ and TCNE in the liquid phase where UV-VIS spectrophotometry was used, while the CT complexes prepared in the solid state were characterized using FT-IR and NMR spectroscopies.
The composition of the complexes was determined by the molar ratio and Job's method. The Benesi-Hildbrand equation was used to calculate the formation constants and the molar extinction coefficient of the CT complexes formed. The new complexes exhibit high formation constant values, suggesting high stability and significant interaction between partners (donor-acceptor). This increased stability is as expected, given the high giving power of the donor and the high electronic affinity of the acceptors. The solvent effect on CT complexes formed in the liquid phase was studied in methanol and ethanol. Additionally, the effect of temperature was studied. revealing that the values of the formation constants increase with increasing temperature.

Keywords: Stelbenoids, Resveratrol, Biodisponibility, CT complexes, Spectroscopy.

Synthèse de quelques dérivés de 3,4-Dihydropyrimidin-2 (1H) -ones portant de fonction sylfonylamide

Tahir HABILA[1,2]*, Mohamed-Zakaria STITI[2], Mourad BOUHEDJA[2] et Smail KHELILI [2].

[1] Higher Normal School of Bousaada, Department of Physical Sciences, 28001 Bousaada, Msila, Algeria
[2] Department of Chemistry, Laboratory of Phytochemistry and Pharmacology, University of Jijel, BP 98 Ouled Aissa, 18000 Jijel, Algeria

✉Corresponding author: habila.tahir@ens-bousaada.dz

Les 3,4-dihydropyrimidinones (DHPMS) sont dotés des propriétés pharmacologiques très intéressantes, touchant plusieurs systèmes biologiques, pouvant les rendre exploitables en thérapie, notamment dans le traitement des maladies cardiovasculaires. L'objectif de ce travail et la synthèse de nouveaux dérivés de 3,4-dihydropyrimidinones portant des restes Sylfonylamide, située en position 4 de l'hétérocycle par une modification structurale de DHPMs élaborées récemment. Cette modification structurale a conduit à une nouvelle série des 'analogues comme c'est illustré dans la Figure 1. Les dérivés des 3,4-dihydropyrimidinone des restes sylfonyl amide ont été préparés en trois étapes. La première étape consiste en la préparation des intermédiaires clé (4a et 4b) suivant la réaction de Biginelli. La deuxième étape est la réduction du groupe nitro porté par le groupe aryle en position 4 de l'hétérocycle pour obtenir les produits intermédiaires (5a, 5b). Enfin, la réaction de condensation du produit 5 avec le sylfonyl acide. Cette condensation mène aux dérivés DHPMs finaux avec de bons rendements à excellent rendements (entre 75 et 90%) et avec un temps de réaction acceptable (20 min à 40 min). La structure des produits finaux et intermédiaires ont été caractérisées par les méthodes d'analyses spectroscopiques (IR, ^{1}H RMN, $_{13}$C RMN), et dont la pureté a été confirmée par l'analyse élémentaire.

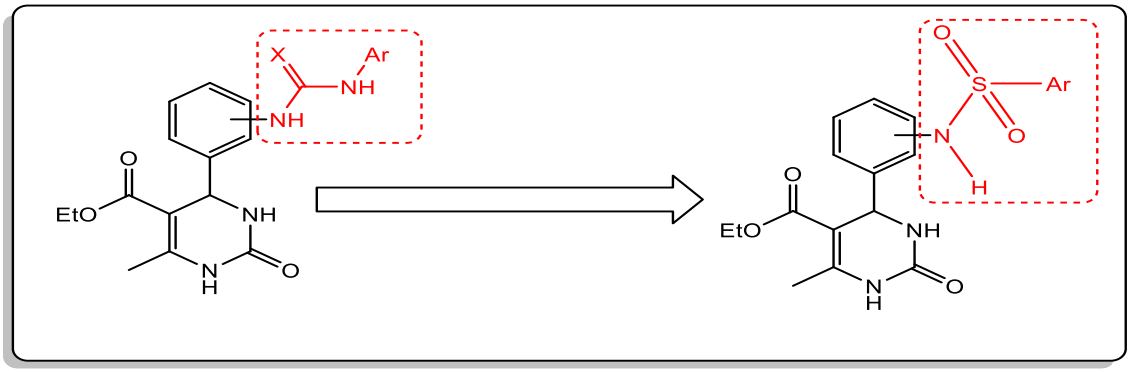

Figure 1: Pharmacomodulation effectuée pour obtenir des nouveaux dérivés de la 3,4-dihydropyrimidinone portant de fonction carbamate.

Mots clés/ (DHPM, Maladies cardiovasculaires, Syfonylamide, Biginelli)

Eggshell and Date Seeds Biochar as a Biostimulant in Food Biotechnology: Modulating the Biochemical and Physiological Traits of Common Bean (Phaseolus vulgaris L)

Malika Hamdiken [1,2], Mehdiya Oumeddour [2], Adama Aliou Fofana [2], Hadia Laouar [3]
[1]Department of Biology, Laboratory of Cellular and Molecular Biology,
University of May 8, 1945, Guelma, Algeria
[2]Department of Biology, University of May 8, 1945, Guelma, Algeria
[3]Department of Ecology, University of May 8, 1945, Guelma, Algeria
Corresponding author: Hamdiken Malika (hamdikenc@yahoo.fr)

Abstract

The objective of this study was to evaluate the effects of soil amendment with biochar on the physiological and biochemical properties of common bean (Phaseolus vulgaris L.). Two types of biochar were tested: one derived from eggshells and the other from date seeds, both applied at different concentrations (1%, 3%, and 5%) to clay soil. The results showed that the addition of biochar significantly enhanced plant growth, with increases in root biomass, leaf area, and stem length. Biochemically, there was an increase in chlorophyll content, total soluble sugars, total proteins, polyphenols, and flavonoids. In parallel, oxidative stress markers such as proline and malondialdehyde (MDA) decreased. Antioxidant activity, assessed using the DPPH (2,2-diphenyl-1-picrylhydrazyl) assay, revealed a notable improvement in radical scavenging capacity, particularly in plants treated with 1% eggshell biochar. Date seed biochar showed marked benefits at 3% and 5% concentrations, whereas eggshell biochar had a stronger impact on photosynthesis and leaf quality. These results confirm that biochar is a promising natural amendment capable of improving soil fertility, enhancing plant stress tolerance, and contributing to sustainable agriculture through the recycling of organic waste.

Keywords: Biochar; Phaseolus Vulgaris L.; soil amendment; eggshells; date seeds; organic waste

Antidiabetic and Antioxydant Effects of Calendula suffruticosa a in an Experimental Model of Diabetes

Hamdiken Malika[1,2], Amina Bouzitouna[3], Ayad Hayette[2], Amara Nardjes[2], Friane Heythem[2], Hamdi Marwa[2], Touahri Raid Abdennour [2]

[1]Department of Biology, Laboratory of Cellular and Molecular Biology, University of May 8, 1945, Guelma, Algeria

[2]Department of Biology, University of May 8, 1945, Guelma, Algeria

[3] Laboratory of Biochemistry and Environment Toxicology, Department of Biochemistry, Faculty of Sciences, Badji Mokhtar University, Annaba 23000, Algeria

Corresponding author: Hamdiken Malika (hamdikene@yahoo.fr)

Abstract

This study aimed to evaluate the antidiabetic and antioxidant properties of a methanolic extract from the Algerian plant Calandula suffruticosa subsp. foliosa). A preliminary phytochemical analysis confirmed the richness of plant in phenolic compounds and its significant in vitro antioxidant activity.

The biological investigation was an experimental study conducted on rats, divided into five groups. Three groups were rendered diabetic via an intraperitoneal injection of streptozotocin (150 mg/kg). One diabetic group was then treated daily with the methanolic extract at a dose of 400 mg/kg. Control groups included untreated diabetic rats, non-diabetic rats, and a diabetic group treated with a reference drug, glibenclamide.

After four weeks of treatment, the results demonstrated that streptozotocin-induced diabetes led to metabolic disorders, hypertension, and an acceleration of oxidative stress markers, alongside a decrease in antioxidant defenses and histological damage to the pancreas and liver.

The methanolic extract of Calandula suffruticosa subsp. foliosa exhibited significant antidiabetic and antioxidant effects. These beneficial actions are likely attributable to its high phenolic content. The extract appeared to protect against free radical damage by reducing lipid peroxidation and by stimulating both enzymatic and non-enzymatic antioxidant defense systems in the diabetic rats.

In conclusion, the findings suggest that this plant extract has therapeutic potential in managing diabetes and associated oxidative stress

Key words: diabetes - phytotherapy - Calendula suffruticosa subsp foliosa (Batt.)-

Oxidative stress.

Molecular Docking and ADMET Prediction of (E)-4-(Phenyldiazenyl) Naphthalen-2(8H) -One

Hibet Errahmane Meroua Akkache[1], Noudjoud Hamdouni[1], Ali Boudjada[1]

[1]Physics Department, Crystallography Laboratory, Constantine University, Constantine, Algeria

Abstract

In this work, we explore the biological potential of (E)-4-(Phenyldiazenyl) naphthalen-2(8H) -one using SwissTargetPrediction. The results suggest that the enzyme 11β-hydroxysteroid dehydrogenase type 1 (HSD11β1) could be a potential biological target.

To validate the docking protocol and identify the active site, we performed a redocking of the native ligand 2-(2-chloro-4-fluorophenoxy)-2-methyl-N-[(1R,2S,3S,5S,7S)-5-(methylsulfonyl)-2-adamantyl] propanamide (NNI) with HSD11β1. The obtained root mean square deviation (RMSD) value was lower than 2 Å, confirming the reliability of the docking protocol. Using the same enzyme and parameters, molecular docking was then performed with our compound.

Finally, ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis was carried out to evaluate the pharmacokinetic and drug-likeness properties, confirming its potential as a promising medical candidate.

Keywords: Docking, Redocking, ADMET, RMSD, HSD11β1

Utilisation des plans d'expériences dans le développement des produits cosmétiques

Imene ABDESSEMED[1], Rihab BENABBAS[2], Abdelhakim ABDESSEMED[3]

1 Université BADJI Mokhtar, faculté des sciences Annaba
2Université BADJI Mokhtar, faculté des sciences Annaba
3Université BADJI Mokhtar, faculté de médecine Annaba
Contact : imeneabdessemed02@gmail.com

Abstract :

Le développement d'un produit cosmétique implique la combinaison de plusieurs ingrédients, chacun jouant un rôle fonctionnel précis, en lien avec la nature du produit fini, sa stabilité (physique, chimique et microbiologique), sa texture (viscosité) ou encore son pouvoir hydratant.
L'optimisation simultanée de ces paramètres requiert souvent la réalisation d'un grand nombre d'expériences, ce qui augmente considérablement le temps et le coût de développement.
L'application des plans d'expériences (Design of Experiments), et plus particulièrement des plans de mélanges, permet au formulateur d'obtenir des résultats à la fois fiables et rapides.
Dans notre étude, nous avons utilisé cette approche pour optimiser la formulation d'un gel douche surgras destiné à apaiser la peau et préserver son confort et son intégrité. Le développement, basé sur l'optimisation des concentrations de trois tensioactifs, n'a nécessité que 12 formules expérimentales.

Après analyse et traitement statistique des résultats, la modélisation de la viscosité a montré une excellente qualité prévisionnelle pour le modèle cubique complet (P-value = 0,0006 ; R^2 ajusté = 0,976116).

La combinaison optimale des tensioactifs a permis d'obtenir une viscosité adaptée, un coût de revient minimal, et une stabilité physique et microbiologique satisfaisante. De plus, la formule finale a passé avec succès les tests d'irritabilité cutanée, confirmant sa tolérance et son efficacité.

Keywords : plans d'expériences, plan de mélanges, produits cosmétiques, gel douche.

Composition Phytochimique D'Urtica dioica L Collecter De La Région De Ain El Arbi (Guelma, Algérie)

Souad KAIDI [(1)], Ismail BOUDEN [(1)], Hanane Nadia BOUSSENANE [1], Hanan BOUKEMARA e[1], Dalila BENDJEDDOU [1] et Mohamed GUETTAF [(2)]

[(1)] Laboratoire de Biologie Moléculaire et Cellulaire, Département de Biologie, Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre et de l'Univers, Université 8 Mai 1945, Guelma, PB 401, 24000, Algérie.

[(2)] Département de Biologie, Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre et de l'Univers, Université 8 Mai 1945, Guelma, PB 401, 24000, Algérie.

KAIDI Souad (souad.kaidi@yahoo.fr)

Résumé

En Algérie, les plantes médicinales sont utilisées depuis longtemps grâce à la richesse et à la diversité de la flore algérienne qui constitue un véritable réservoir phylogénétique, avec environ 3000 espèces appartenant à plusieurs familles botaniques. Parmi les plantes mondialement connues pour leurs effets bénéfiques ; Urtica dioica L, communément appelée ortie. Elle est utilisée en médecine traditionnelle dans le traitement de plusieurs maladies telles que : la néphrite, la jaunisse, les hémorragies, l'arthrite et les rhumatismes et elle possède également des effets antibactériens, antioxydants et analgésiques. Ce travail consiste à effectuer des tests phytochimiques de l'extrait aqueux d'Urtica dioica L, préparé à partir de la partie aérienne de la plante afin d'évaluer la composition chimique en métabolite secondaire de cette plante.

Les résultats des tests phytochimiques réalisés sur le matériel végétal broyé et l'extrait aqueux d'Urtica dioica L montrent :

- La présence des teneurs importante de flavonoïdes, de terpanoides, de quinones, et de saponosides.
- La présence des teneurs moyennes de tanins et de anthocyanes.
-La présence des teneurs faible de coumarines et de mucilages
- L'absence des teneurs en alcaloïde.

Mots clés : Plante médicinale, Urtica dioica, tests phytochimiques, Guelma

A Comparative Study on The Antioxidant Properties of Epigallocatechin Gallate, Epicatechin, Resveratrol, And Ascorbic Acid

Karima Belguidoum[1], Yamina boulmokh[1], Mouna Nacef [2], Hanane Messiad[1, 3], Hayet Belbah[1], Fatima Zahra Hamamdia[1], Aïda Rebaïa Nadji[2], Nadjette Bengourna[4] and Habiba Amira-Guebailia[1]

[1]Laboratoire de Chimie Appliquée -LCA, Université 8 Mai 1945 Guelma, BP 401, Guelma 24000, Algeria.

[2]Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université 8 Mai 1945 Guelma, BP 401, Guelma, 24000, Algeria.

Université de Constantine 3, Algeria.

[3]Laboratoire des Silicates, Polymères et des Nanocomposites (LSPN), Université 8 Mai 1945, Guelma, BP 401, Guelma, 24000, Algeria.

Email: belguidoum.karima@univ-guelma.dz

Abstract

This study investigates and compares the antioxidant activity of two green tea polyphenols, epigallocatechin gallate (EGCg) and epicatechin (EC), with those of the reference antioxidants resveratrol (RSV) and ascorbic acid (AA). Two well-established assays were employed: DPPH free radical scavenging and FRAP (Ferric Reducing Antioxidant Power). RSV and AA served as standard references to allow direct assessment of antioxidant efficiency. According to the FRAP assay, EGCg exhibited a strong ability to reduce Fe^{3+} ions, particularly at low concentrations. Results from the DPPH assay confirmed that EGCg displayed higher antiradical activity than RSV but lower than AA. Overall, the order of antioxidant potency based on IC50 values was AA > EGCg > EC > RSV.

Keywords: Antioxidant, DPPH, FRAP, EGCg, RSV, Ascorbic acid.

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Étude in silico de l'interaction de flavonoïdes naturels avec des cibles enzymatiques impliquées dans la résistance antibactérienne : Approche combinée de reverse screening et docking moléculaire

L. Karoun [1], S. Aitkaki [2], F. Layachi[3], A. Neghra [4]
Laboratoire de Chimie Thérapeutique, département de Pharmacie, Faculté de Médecine, UBMA

E-mail : karounlidia92@gmail.com

La résistance antibactérienne constitue un défi majeur pour la santé publique mondiale, soulignant le besoin urgent de nouvelles molécules inhibitrices. Les flavonoïdes, composés polyphéniques naturels, présentent un potentiel thérapeutique en ciblant des enzymes clés de la résistance bactérienne, telles que les β-lactamases et les pompes à efflux. **L'objectif de cette étude est d'identifier et d'évaluer in silico des flavonoïdes naturels capables d'inhiber ces enzymes, afin de proposer de nouveaux candidats thérapeutiques.**

Un panel de flavonoïdes a été sélectionné depuis la base PubChem. Le reverse screening, via SwissTargetPrediction et PharmMapper, a permis de prédire les cibles enzymatiques potentielles. Les structures cristallographiques des enzymes cibles ont été récupérées dans PDB, nettoyées et préparées pour le docking moléculaire avec Molegro Virtual Docker. Le docking a évalué l'affinité et la stabilité des complexes ligand-enzyme, tandis que l'analyse des interactions a identifié les liaisons hydrogène, hydrophobes et π-π importantes pour l'inhibition.

Les résultats montrent que plusieurs flavonoïdes présentent une affinité significative pour les enzymes ciblées, avec des interactions stables sur les sites actifs. Les scores de docking et de re-rank suggèrent une inhibition compétitive potentielle, indiquant que ces molécules peuvent agir comme inhibiteurs efficaces. Cette étude démontre que la combinaison de reverse screening et de docking moléculaire est une approche efficace pour la découverte rapide de candidats naturels contre la résistance antibactérienne, offrant une base solide pour des validations expérimentales ultérieures et la conception de nouvelles stratégies thérapeutiques.

Mots-clés : Flavonoïdes, résistance antibactérienne, docking moléculaire, reverse screening, inhibition enzymatique.

Extraction en Phase Solide d'un Métabolite Urinaire du Benzène : Valorisation des Propriétés Acido-basiques

Fazia KERKOUB [1,2], Rachid DJAFER [1,2]

[1]Laboratoire de Toxicologie Médicale, Département de Pharmacie, Faculté de Médecine, Université Badji Mokhtar, Annaba, Algérie
[2]Laboratoire de Toxicologie, CHU Ibn Sina, Annaba, Algérie

Auteur correspondant : Fazia KERKOUB (fazia.kerkoub@univ-annaba.dz)

Résumé

L'acide trans, trans-Muconique (t,t-MA) est un métabolite urinaire minoritaire du benzène, dosé dans le cadre de la surveillance professionnelle de l'exposition des travailleurs à ce dernier. Avant l'analyse par chromatographie liquide à haute performance, une extraction est nécessaire afin d'enrichir l'analyte et améliorer la détection. Nous avons développé une technique d'extraction en phase solide (SPE) du t,t-MA à l'aide de cartouches de type SAX (Strong Anion Exchange) greffées avec des groupes quaternaires d'ammonium (chargés positivement) et conçues pour retenir les analytes chargées négativement notamment les acides faibles. La rétention se fait par interaction électrostatique entre la phase stationnaire et les analytes anioniques. Le défi est de choisir la composition, le volume et le débit des solvants afin d'assurer une meilleure fixation de l'analyte d'intérêt avec un bon lavage des impuretés, puis un bon rendement lors de la phase finale d'élution pour assurer un meilleur rendement. Nous avons optimisé le pH des urines, et utilisé différentes concentrations de l'acide acétique entre les différentes étapes de la SPE. Le rendement est entre 97% et 100%. Les liquides de la phase du dépôt, lavage et élution étaient constamment analysés par HPLC-DAD afin de vérifier les éventuelles pertes.

Mots clés : métabolite urinaire, acide trans, trans-muconique, extraction en phase solide, acide faible, cartouches SAX

Analyse Qualitative Des Métabolites Secondaires Du Tournesol Helianthus annuus Cultivé En Algérie

Khedidja Amira[1,2], Nour El-Houda Djeghader[2,3], Meriem Snani[1]

[1] Departement des Sciences naturelles, Ecole Normale Supérieure de l'Enseignement Technologique- Skikda, Algérie
[2]Laboratoire de Physique, Chimie et Biologie des matériaux, ENSET- Skikda, Algérie.
[3]Departement de Biologie, Faculté des Sciences, Université BADJI Mokhtar- Annaba, Algérie.
Corresponding author: Khedidja Amira (amira_khedidja@yahoo.com)

Résumé

Le tournesol appartient à la famille des Astéracées, au genre Helianthus et à l'espèce annuus. Le genre Helianthus comprend environ 70 espèces, dont deux sont cultivées pour la consommation humaine et animale : H. annuus (tournesol) et H. tuberosus. Le tournesol est une plante annuelle de grande taille, dotée d'une tige solide et légèrement ramifiée pouvant atteindre jusqu'à 4 mètres de hauteur. Son huile, utilisée seule ou en combinaison avec d'autres, répond à divers besoins de l'industrie agroalimentaire. Utilisée seule, l'huile de tournesol entre dans la préparation de sauces, de vinaigrettes et pour la friture ; cependant, elle est particulièrement précieuse lorsqu'elle est mélangée à d'autres huiles à des fins nutritionnelles. Cette étude vise à identifier certains composés chimiques bioactifs, appelés métabolites secondaires, tels que les saponines, les tanins, les flavonoïdes, les alcaloïdes et les terpènes, présents dans la plante Helianthus annuus cultivé à Annaba, à l'aide d'un extrait aqueux de graines moulues. Les résultats ont révélé la présence de saponines (indiquée par la formation d'une mousse stable), de tanins, de flavonoïdes et d'alcaloïdes (observée par des changements de couleur), et l'absence de terpènes dans l'extrait aqueux de graines utilisé. Ces composés sont connus pour conférer diverses propriétés thérapeutiques à la plante étudiée.

Mots clés : Astéracées, Helianthus annuus, métabolites secondaires, extrait aqueux, graines, propriétés thérapeutiques.

Redox Profiling of an Arid Desert Plant Using the Cupric Ion Reducing Antioxidant Capacity (CUPRAC) Assay

Amel KHEROUF [1]*, Marwa KHEROUF[1], Imen TEBBOUB[1]

[1] Department of Biochemistry, Laboratory of Microbiology and Molecular Biology, Department of Biochemistry, University of Badji Mokhtar, Annaba, Algeria

Corresponding author: kheroufamel1@gmail.com

Abstract

Many Saharan plants, valued in traditional medicine, have yielded important compounds like morphine, opium, and anesthetic alkaloids. These plants may serve as reservoirs of natural, safe, and effective antioxidant macromolecules. The study examines Ephedra alata, an ancient medicinal plant renowned for its numerous therapeutic properties, which is typically found in arid and semi-arid regions. The main objective of this study is to identify the phytochemical compounds in the methanolic extract of Ephedra alata subsp. alenda and to quantify its total polyphenols and flavonoids. Furthermore, the antioxidant activity of this extract was assessed using the DPPH radical scavenging assay, the ferric reducing antioxidant power (FRAP) assay and cupric ion reducing antioxidant capacity (CUPRAC). Phytochemical analysis confirmed the presence of tannins, saponins, alkaloids, phenolic compounds, and anthocyanins. The concentrations of total polyphenols, flavonoids, and tannins were found to be 320.5 ± 6.16 µg GAE/mg, 96.86 ± 2.5 µg QE/mg, and 60.54 ± 8.91 µg EC/mg, respectively. The extract demonstrated antioxidant potential, exhibiting a reducing capacity of 147.5 µmol TE/g toward Cu^{2+} ions, while the IC_{50} values in the DPPH and FRAP assays were 41.5 ± 2.06 µg/mL and 6.63 ± 0.01 µg/mL, respectively. In conclusion, these findings emphasize the strong antioxidant potential of Ephedra alata subsp. alenda, supporting its traditional medicinal use and pointing to its potential applications in pharmacology and nutrition.

Keywords : Saharan plants, CUPRAC, tannins, Cu^{2+}, antioxidant potential

Synthèse, caractérisation et évaluation de l'activité antiacide d'une poudre d'hydroxyde de magnésium à usage pharmaceutique

Leila Mekahlia[a] *, Radia Mekahlia[b], Amina Labouiz[c], Youcef Hadef [C], Abdelali Merah [A]

[a] Laboratoire de Chimie Minérale, Département de Pharmacie, Faculté de Médecine, Université BADJI Mokhtar 23000 Annaba
[b] Laboratoire central, Etablissement Public Hospitalier El Hadjar, Annaba
[c] Laboratoire de développement et de contrôle de préparations pharmaceutiques hospitalières, Département de Pharmacie, Faculté de Médecine, Université BADJI Mokhtar 23000 Annaba

E-mail : mekahlialeila@hotmail.fr

Résumé

Le présent travail s'inscrit dans le cadre de la recherche appliquée visant à développer des solutions thérapeutiques locales à partir de matières premières accessibles. Il a porté sur la synthèse, la caractérisation et l'évaluation de l'activité antiacide d'une poudre d'hydroxyde de magnésium ($Mg(OH)_2$), un composé largement utilisé en thérapeutique gastro-intestinale pour ses propriétés antiacides et laxatives dépendant de la dose.

La synthèse a été réalisée à partir d'une solution alcaline et d'une solution de nitrate de magnésium (ratio 50 %), conduisant à une poudre blanche, fine et amorphe, pratiquement insoluble dans l'eau, avec un rendement de 99,7 %. Les essais d'identification qualitative (réaction au phosphate disodique) ont confirmé la présence du magnésium, tandis que les analyses quantitatives ont démontré une pureté conforme à la Pharmacopée Européenne : chlorures < 0,15 %, sulfates < 1 %, calcium < 1,5 %, fer < 0,07 %, perte à la calcination de 30 %. Les analyses complexométriques et infrarouges (IR) ont validé la structure caractéristique du $Mg(OH)_2$. Le dosage (87,48 mg pour 0,1 g) confirme la conformité du produit synthétisé. L'étude de l'activité antiacide, conduite par méthodes pH-métrique et titrimétrique, a révélé une capacité de neutralisation rapide et efficace, comparable à certains antiacides commerciaux, bien que légèrement inférieure aux formulations combinées.

Ces résultats démontrent la faisabilité technique d'une production locale d'hydroxyde de magnésium de qualité pharmaceutique, offrant une alternative crédible et économique pour le traitement de l'hyperacidité gastrique et la constipation occasionnelle.

Mots-clés : hydroxyde de magnésium, synthèse, caractérisation, activité antiacide, contrôle qualité, pharmacopée.

Évaluation comparative de la capacité de neutralisation acide des antiacides commercialisés en Algérie

Leila MEKAHLIA[a] *, Amina LABOUIZ[b], Radia MEKAHLIA[c], Youcef HADEF [b], Abdelali MERAH [a]

[a]Laboratoire de Chimie Minérale, Département de Pharmacie, Faculté de Médecine, Université BADJI Mokhtar 23000 Annaba
[b]Laboratoire de développement et de contrôle de préparations pharmaceutiques hospitalières, Département de Pharmacie, Faculté de Médecine, Université BADJI Mokhtar 23000 Annaba
[c] Laboratoire central, Etablissement Public Hospitalier El Hadjar, Annaba

E-mail: mekahlialeila@hotmail.fr

Résumé

L'hyperacidité gastrique, résultant d'une sécrétion excessive d'acide chlorhydrique, constitue une cause majeure de troubles digestifs tels que le reflux gastro-œsophagien et la dyspepsie. Les médicaments antiacides, principalement composés de sels minéraux (hydroxydes ou carbonates de calcium, magnésium et aluminium), agissent par neutralisation de l'excès d'acidité. Cette étude vise à comparer la capacité de neutralisation acide (ANC) de treize antiacides disponibles sur le marché algérien et à évaluer leur conformité aux normes de la Food and Drug Administration (FDA) et de la United States Pharmacopeia (USP). L'ANC a été déterminée par titrage en retour selon deux méthodes : pH-métrique et titrimétrique, conformément aux spécifications de l'USP.
Les résultats révèlent que la majorité des échantillons présentent une ANC supérieure aux valeurs minimales recommandées, à l'exception de deux formulations. Les antiacides à base de carbonates de calcium et de magnésium (ex. Rennie, Maalox) ont montré les meilleures performances, tandis que les formes liquides se distinguent par une neutralisation plus rapide et plus efficace. Une corrélation directe entre la teneur en principes actifs et l'ANC a été observée. Les antiacides contenant de l'alginate et du bicarbonate, bien que moins puissants sur le plan chimique, offrent un mécanisme complémentaire de protection mécanique du reflux acide. Ces résultats mettent en évidence l'importance de la composition et de la forme galénique dans l'efficacité neutralisante, et soulignent la nécessité d'une harmonisation des critères d'évaluation au sein des pharmacopées.

Mots-clés : Antiacides, Capacité de neutralisation acide, Hyperacidité gastrique, Sels minéraux.

Synthesis and Spectroscopic Characterization of a Phenolic Schiff Base

Manal CHETTIBI[1], Saida SERIDI [2]

[1,2] Laboratory of Physical Chemistry, University of 8 Mai 1945, BP 401, Guelma, Algeria
Corresponding author: Manal CHETTIBI (chettibi.manal@univ-guelma.dz)

Abstract

The research in the present study carried out the synthesis of Schiff base ligand, 2,2'-{benzene-1,4-diylbis[nitrilo(E)methylylidene]} diphenol from reaction of salicylic aldehyde with para-phenylenediamine. The reaction generated a symmetrical and conjugated ligand, which has phenolic groups and imine linkages. This lead to a ligand with various metal coordination sites. We studied the ligand with infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy. IR studies confirmed the presence of characteristic imine stretching vibrations between 1600 and 1650 cm^{-1}. The UV-Vis spectra showed $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, indicating extended conjugation and possible electron donation. The e-vidence proposed indicates a strong chelating ability and electronic versatility of ligand that can efficiently form complexes with TMs.

Keywords : Schiff base, Infrared, Ultraviolet-visible.

Antioxidant Activity of Dichloromethane Extract Using Ultrasound assisted Extraction from Umbilicus Rupestris Leaves Plant

Nessrine Marhoune [1], Souad Ameddah [2], Ahmed Menad [2] Amel Moussaoui [3] chourouk[4] Babouche

[1] Departement of biochemistry and Molecular and cellular Biology, Faculty of Natural and Life Sciences, Mentouri brother's University 1. Biology and Environment Laboratory, Algeria.

[2]Department of Animal Biology, Faculty of Natural and Life Sciences, Mentouri brother's University 1. Biology and Environment Laboratory, Algeria.
[3]Department of applied biology, Faculty of Natural and Life Sciences Echahid Echikh Larbi University of Tebessa, Algeria.
[4] Abbes Laghrour University, Faculty of Natural and Life Sciences, Khenchela, Algeria.
Corresponding author: nesrine.marhoune@umc.edu.dz

Abstract

Medicinal plants have been used by people since antiquity to treat a variety of illnesses, as scientific progress has shown that active substances such as the polyphenols present in these plants have an antioxidant effect. antioxidants have been traditionally used as well as experimentally proved beneficial. The antioxidant components of the natural products constitute the major source of human health promotion and maintenance [1] The aim of this work is to evaluate the antioxidants activities of dichloromethane extract. The extraction of plant materials was performed using ultrasound, (vibra cell 75186),10 g of plant powder was mixed with 100 ml of solvent, this mixture was then sonicated for 30 min at 40°c and 40 kH frequency. The antioxidant activities of ethyl acetate extract obtained from Umbilicus rupestris leaves, collected during the flowering period, were evaluated and to investigate this potential, extract were tested on their capacity to react with diphenyl-picrylhydrazyl (DPPH), 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid (ABTS), Reducing power (RP) and O-Phenanthroline Chelating Activity. The results showed strong antioxidant activity, in the case of the hydrogen proton transfer methods (DPPH, ABTS), and in the electron transfer methods (Reducing Power and O-Phenanthroline Chelating Activity). Respectively: 24,76±0,06mg TROLOX/100 g DW, 22,56±1,12mg TROLOX/100 g DW, 75,14±0,17mg TROLOX/100 g DW and 48,34 mg TROLOX/100 g DW. In conclusion, the Dichlomethane extract from Umbilicus rupestris leaves has an antioxidant propriety, Due to the plant's richness in polyphenols.

Keywords: Antioxidant; Dichloromethane, Umbilicus rupestris.

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Bunium sp. and the Secrets of Solvents: A Dual Impact on Bioactivity and Health

Amel Moussaoui [1], Samira Boussekine [1], Nesrine Marhoune [2], Chourouk Babouche [3]

[1] Department of Applied Biology, Laboratory of Bioactive Molecules and Applications, Echahid Echikh Larbi University of Tébessa, Tébessa, Algeria.

[2] Department of Biochemistry and Molecular and Cellular Biology, Biology and Environment Laboratory, Frères Mentouri University Constantine 1, Constantine, Algeria.

[3] Department of Molecular and Cellular Biology, Laboratory of Biotechnology, Water, Environment and Health University of Abbes Laghrour, Khenchela, Algeria.

moussaouiamel12@gmail.com

Abstract

Behind every plant extract lies a complex interplay between the solvent, the metabolite, and the working environment. In studies focusing on Apiaceae species, particularly Bunium sp., extraction solvents play a dual role: they determine the chemical composition and bioactivity of the extracts while also potentially affecting the health of laboratory personnel handling these substances. Several studies have demonstrated that the choice of solvent alters the polarity of recovered metabolites and thus their biological activity (Khoddami et al., 2013; Do et al., 2014). Polar solvents such as methanol and ethanol tend to extract more phenolic and antioxidant compounds, whereas non-polar solvents favor lipidic and terpenic fractions. However, certain extracted substances may degrade or lose stability depending on the solvent used, thereby influencing their therapeutic efficacy (Chemat et al., 2017). Moreover, chronic exposure to laboratory solvents has been associated with toxic effects, including neurological and hepatic impairments (Bahadar et al., 2014). This work proposes an interdisciplinary reflection at the crossroads of phytochemistry, toxicology, and occupational health, emphasizing the need for a transition toward safer and greener extraction processes.

Keywords: Bunium sp., extraction solvents, toxicity, laboratory safety.

From Plant to Molecule: Decoding the Green Chemistry of Apiaceae through Ultrasound and Infrared Light.

Moussaoui Amel[1], Boussekine Samira[1], Marhoune Nesrine[2], Babouche Chourouk[3]

[1] Department of Applied Biology, Laboratory of Bioactive Molecules and Applications, Echahid Echikh Larbi University of Tébessa, Tébessa, Algeria.
[2] Department of Biochemistry and Molecular and Cellular Biology, Biology and Environment Laboratory, Frères Mentouri University Constantine 1, Constantine, Algeria.
[3] Department of Molecular and Cellular Biology, Laboratory of Biotechnology, Water, Environment and Health University of Abbes Laghrour, Khenchela, Algeria.
moussaouiamel12@gmail.com

Abstract

The Apiaceae family comprises numerous species recognized for their richness in secondary metabolites with high pharmaceutical potential. In this context, the present study aimed to establish a reliable and efficient methodology for the extraction and functional characterization of bioactive compounds from a local species belonging to this family. Underground parts were dried, finely powdered, and subjected to ultrasound-assisted extraction (UAE) at a 1:10 (w/v) ratio for 30 minutes at 40 °C and 50 kHz using four solvents: 70% ethanol, hexane, chloroform, and petroleum ether. This environmentally friendly and rapid technique enables efficient recovery of metabolites while preserving thermosensitive compounds. Functional characterization was carried out using Fourier Transform Infrared (FTIR) spectroscopy, a non-destructive and rapid analytical method, which revealed characteristic absorption bands attributed to hydroxyl, carbonyl, aromatic, and aliphatic groups. These findings confirm the coexistence of phenolic and terpenic fractions, typical of Apiaceae species, and highlight the relevance of the UAE–FTIR combination as a green and rapid approach to guide future chromatographic and spectrometric phytochemical investigations.

Keywords: Apiaceae, Ultrasound-Assisted Extraction, FTIR.

Ni (II)–Hapc complexes against fungal exo-β-(1,3)-glucanase: brief crystallographic context and a docking-focused evaluation

Nour El Houda GUERAH[1], Ouided Benslama[2], Sofiane BOUACIDA[3,4], Rafika BOUCHENE[5].

[1] Laboratoire des Sciences Analytiques, Matériaux et Environnement, Université Larbi Ben M'Hidi, Oum El Bouaghi 04000, Algeria
[2] Laboratoire des Substances Naturelles, Biomolécules et Applications Biotechnologiques, Département des Sciences de la Nature et de la Vie, Université Larbi Ben M'Hidi, Oum El Bouaghi 04000, Algérie.
[3] Département Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Université Larbi Ben M'Hidi, Oum El Bouaghi, Algeria.
[4] Unité de recherche de Chimie Moléculaire et Structurale CHEMS, Université Constantine 1, 25000, Algérie.
[5] Laboratoire des Sciences Analytiques, Matériaux et Environnement, Université d'Oum El Bouaghi, Oum El Bouaghi 04000, Algérie.

Abstract

Ni (II) complexes formed with 3-aminopyrazine-2-carboxylate (Hapca) were prepared in mild conditions and structurally established by single-crystal X-ray diffraction (κ^2N, O chelation around octahedral Ni (II)); this brief crystallographic context was used to build reliable 3D inputs for molecular modeling. Here we concentrate on the docking study featured in the thesis: the hydrated and anhydrous forms (Ni1, Ni2) were geometry-prepared from their CIF-derived structures and energy-minimized (MMFF94), then docked with AutoDock Vina into the catalytic pocket of the exo-β-(1,3)-glucanase (Exg) from Candida albicans. Both Ni complexes achieved favorable binding poses and scores compared with the parent ligand (Hapca), consistent with the observed in vitro trends. The best poses are stabilized by a network of hydrogen bonds and hydrophobic/van der Waals contacts inside the Exg gorge; residue-level analysis indicates H-bonding for Ni1 with active-site residues and, for Ni2, contacts involving Phe^{144} and Trp^{363}, among others. Pose quality was assessed by internal convergence of top-ranked solutions. Taken together, these results support the plausibility of Exg engagement by Hapca–Ni (II) scaffolds and motivate enzyme assays and structure-guided optimization.

Keywords: nickel (II); Hapca; exo-β-(1,3)-glucanase; Candida albicans; molecular docking; AutoDock Vina.

Metal-Drug Interactions between Oral Antidiabetics (Glibenclamide, Gliclazide, Glimepiride) and Biometals: Chemical Insights and Applied Perspectives

Hassina Fisli [1], Mohamed Lyamine Chelaghmia [2]

[1] Material sciences department, Laboratory of Applied Chemistry (LCA), 8 mai 1945 Guelma University, Guelma, Algeria
[2] Process Engineering Department, Materials analysis and engineering laboratory (LAIGM), 8 mai 1945 Guelma University, Guelma, Algeria
Corresponding author: Fisli Hassina (fisli.hassina@univ-guelma.dz)

Abstract

Type 2 diabetes mellitus represents one of the most prevalent chronic diseases worldwide, requiring effective and sustainable therapeutic approaches. Oral antidiabetics such as glibenclamide, gliclazide, and glimepiride are key sulfonylurea derivatives used to achieve glycemic control. From a chemical perspective, these molecules contain functional groups capable of coordinating with biologically important metal ions such as Mn^{2+}, Fe^{2+}, and Co^{2+}. The formation of metal–drug complexes can alter essential physicochemical parameters including solubility, stability, and molecular conformation, thereby influencing the bioavailability and pharmacological performance of the drugs. The investigation of these interactions through spectroscopic techniques allows the identification of coordination sites and provides insight into the binding mechanisms. Such studies are crucial for understanding the impact of metal ions on drug behavior under physiological conditions and for predicting possible modifications in therapeutic efficacy or toxicity. Furthermore, this research aligns with the goals of green and sustainable chemistry. Optimizing the synthesis and stability of metal–drug complexes contributes to reducing waste generation and minimizing the environmental footprint of pharmaceutical production. Therefore, the study of interactions between oral antidiabetic drugs and biometals offers an interdisciplinary approach that bridges analytical chemistry, pharmaceutical research, and sustainable development, paving the way for safer, more efficient, and environmentally responsible therapeutic strategies.

Keywords: Oral antidiabetics, Metal–drug complexes, Spectroscopic analysis, Coordination chemistry

Synthèse, Caractérisation et Evaluation de L'activité Biologique de deux Nouveau Imines

Ouafa Boukhemis [1,2], Naouel Boudraa [1] Mohamed Sallah Benlatreche [3]

[1]Centre de recherche en biotechnologie (CRBT) Ali Mendjili nouvelle ville UV 03 BP E73 Constantine. Algérie.
[2]Unite de Recherche Chimie de l'Environnement et Moléculaire Structurale 'CHEMS', Faculté des Sciences Exactes, Campus Chaabet Ersas, Université Constantine 1, 25000 Constantine, Algérie.
[3]Directeur du Laboratoire de Génie et Technologies de l'Environnement, Centre Universitaire Abdelhafid Boussouf de Mila, Algérie.
Auteur E-mail: Wafa2535@gmail.com

Résumé :

Dans ce travail, nous avons synthétisé deux nouvelles imines par réaction de condensation, obtenues avec d'excellents rendements. La structure de ces bases de Schiff a été déterminée par diffraction des rayons X sur monocristal.
Plus précisément, les bases de Schiff ont été préparées à partir de la 3,3'-diméthoxybenzidine et du 4-nitrobenzaldéhyde, ainsi que du 5-bromobenzaldéhyde.
Les structures cristallines des deux composés obtenus ont été confirmées par diffraction des rayons X à monocristal.
Les données cristallographiques ont été collectées à l'aide d'un diffractomètre Xcalibur, Atlas, Gemini, avec les paramètres de maille suivants :
Composé 1 :a = 8,6304 Å, b = 20,6176 Å, c = 26,9165 Å, α = 90°, β = 90°, γ = 90°.
Composé 2 :a = 14,7893 Å, b = 4,8765 Å, c = 27,3458 Å, α = 90°, β = 90°, γ = 90°.
L'objectif principal de cette étude est d'évaluer les activités antioxydantes de deux molécules synthétisées, à travers trois essais : le piégeage des radicaux libres DPPH, le piégeage des radicaux cationiques ABTS et l'essai CUPRAC.

Mots clés: Imine, Synthèse chimique, diffraction des rayons X, activité antioxydant.

Antimicrobial, Antioxidant and Anti-inflammatory Properties of 3-(2-chloroacetyl) oxazolidin-2-one New Synthesis: Molecular Docking and DFT Study

Radia BOUASLA[1,2], Malika BERREDJEM[1], Khadidja OTMANE RACHEDI[1,3], Seif-Eddine DJOUAD[1], Manel Lina DJENDI[4], Chahrazed BENZAID[4]

[1]Laboratory of Applied Organic Chemistry, Synthesis of Biomolecules and Molecular Modelling Group, Department of Chemistry, Sciences Faculty, Badji-Mokhtar-Annaba University, Box 12, 23000 Annaba, Algeria.
[2]Higher School of Industrial Technologies-Annaba, Box 218, 23000 Annaba, Algeria.
[3] University El-Tarf, Alger, Algeria.
[4]Laboratory of Microbiology and Molecular Biology, Badji-Mokhtar Annaba University, Box 12, 23000. Annaba, Algeria.
Corresponding author: Radia BOUASLA (r.bouasla@ensti-annaba.dz)

Abstract

Antibiotics play a crucial role in modern medicine, significantly reducing the impact of infectious diseases. However, the increase in antibiotic resistance represents a significant challenge, especially considering the obstacles to developing new drugs. In this regard, Oxazolidinones, a class of five-member heterocyclic compounds, have shown great promise in various therapeutic areas. In addition, new oxazolidinone derivatives have been synthesized and tested for their antimicrobial efficacy, showing promising results against Gram-positive pathogens, including Bacillus subtilis and Streptococcus pyogenes.

In this work, we investigate the potential of a newly synthesized oxazolidinone molecule; 3-(2-chloroacetyl) oxazolidinones, to inhibit the growth of various pathogen microorganisms. We explore its potential to inhibit the growth of Gram-positive and Gram-negative bacteria and yeasts of the genus Candida in both planktonic and biofilm modes. A molecular docking study was carried out to understand better and research the mechanisms of action. In terms of antioxidant capacity, the molecule tested showed a (2, 2-diphenyl-1 picrylhydrazyl) (DPPH) scavenging activity with an IC50 value of 5.58 ± 0.02 µg/mL, and an anti-inflammatory effect demonstrated a percentage inhibition of about 84.38 ± 5.11%. For the HOMO-LUMO analysis, the compound has a positive log p-value, confirming its lipophilicity and biological activity.

Keywords: Antibiotics, Oxazolidinones, antioxidant capacity, anti-inflammatory.

Impact de l'hyperbilirubinèmie (ictère) sur le dosage de la créatinine plasmatique

Radia MEKAHLIA, Yazila MANCER

[a] Laboratoire central, Etablissement Public Hospitalier El Hadjar, Annaba

E-mail : radiamekahlia@gmail.com

La créatinine est un marqueur essentiel de la fonction rénale, son dosage est souvent réalisé par la méthode de Jaffé (colorimétrique) ou enzymatique. L'ictère peut interférer avec ces dosages en modifiant la lecture spectrophotométrique (sous-estimation selon la méthode utilisée).

L'objectif de ce travail est d'évaluer l'influence de l'ictère (hyperbilirubinémie) sur le dosage de la créatinine sérique selon la méthode utilisée sur l'automate de biochimie.

Une étude comparative a été réalisée sur des échantillons sériques présentant différents niveaux de bilirubine. La créatinine a été dosée par la méthode Jaffé cinétique et la méthode enzymatique (référence).

Les échantillons ont été classés selon le degré de l'ictère (léger, modéré, sévère). Les écarts de résultats entre les deux méthodes ont été analysés.

Une corrélation négative a été observée entre la concentration de bilirubine et créatinine mesurée par la méthode Jaffé. Les valeurs de créatinine étaient significativement sous estimées dans les sérums ictériques. En revanche, la méthode enzymatique est restée peu influencée par la bilirubine jusqu'à des concentrations élevées.

L'ictère interfère significativement avec le dosage de la créatinine par la méthode de Jaffé, entrainant une sous-estimation des résultats. Il est donc recommandé d'utiliser la méthode enzymatique chez les patients ictériques pour une évaluation plus fiable de la fonction rénale.

Mots-clés : Créatinine, Ictère, Interférence, Méthode Jaffé, Méthode enzymatique.

Élaboration et caractérisation des nanoparticules d'oxyde de zinc (ZnO) à usage antimicrobien

Radia MEKAHLIA [a] *, Abdelali MERAH [b], Samia BOULEDROUA[b], Leila MEKAHLIA[b]

[a]Laboratoire central, Etablissement Public Hospitalier El Hadjar, Annaba
[b]Laboratoire de Chimie Minérale, Département de Pharmacie, Faculté de Médecine, Annaba

E-mail: radiamekahlia@gmail.com

Les nanoparticules d'oxyde de zinc (ZnO) suscitent un intérêt croissant en raison de leurs propriétés physico-chimiques remarquables et de leurs multiples applications biomédicales et industrielles. Elles sont notamment utilisées comme agents antimicrobiens, supports de vectorisation de principes actifs, filtres UV dans les écrans solaires ou encore additifs fonctionnels dans divers produits pharmaceutiques et cosmétiques.

L'objectif de ce travail est l'élaboration de nanoparticules de ZnO pur et leur caractérisation par des techniques structurales, morphologiques et spectroscopiques. Les nanoparticules ont été synthétisées par la méthode de précipitation, puis caractérisées par spectroscopie UV-Visible, spectroscopie infrarouge à transformée de Fourier (FT-IR), microscopie électronique à balayage (MEB) couplée à la spectroscopie dispersive d'énergie (EDS), et diffraction des rayons X (DRX).

L'analyse optique (UV-Vis) a révélé un maximum d'absorbance à 379,88 nm, confirmant la formation du ZnO. Les spectres FT-IR ont mis en évidence les bandes caractéristiques des liaisons métal-oxygène (Zn–O). L'observation MEB a montré des particules sphéroïdales de taille nanométrique, tandis que l'analyse EDS a confirmé une pureté chimique élevée. Les diagrammes de DRX ont révélé une structure cristalline hexagonale de type wurtzite, avec une taille moyenne de cristallites de 54,5 nm.

Ces résultats démontrent que la méthode de précipitation permet d'obtenir des nanoparticules de ZnO de bonne pureté, à faible coût, et présentant un fort potentiel pour des applications antimicrobiennes.

Mots-clés : nanoparticules, oxyde de zinc, précipitation, caractérisation, propriétés antimicrobiennes.

Caractérisation des métabolites bioactifs de Pleurotus ostreatus et évaluation de ses propriétés nutritionnelles

Zahra Razkallah [1,2*], Sana Abdellioui.[1,2], Amina Doghmane. [1,2], Nariman Aounallah. [1], Wahiba Hemaizia. [1], Moussa Houhamdi [1,2]

1: Université 8 Mai 1945 Guelma

2: Laboratoire de Biologie, Eau et Environnement (LBEE), Faculté des Sciences de la Nature et de la Vie et des Sciences de la Terre et de l'Univers, Université 8 Mai 1945 Guelma

zahra.razkallah@yahoo.fr

Résumé

Les champignons comestibles constituent une source importante de nutriments et de composés bioactifs, leur conférant un intérêt croissant dans les domaines nutritionnel et pharmaceutique. Parmi eux, Pleurotus ostreatus est largement étudié pour sa richesse en métabolites secondaires et en macronutriments, susceptibles de contribuer à ses propriétés biologiques. L'objectif de ce travail est de caractériser la composition phytochimique et biochimique de l'extrait brut de Pleurotus ostreatus, en mettant en évidence ses principaux constituants et en évaluant leurs teneurs respectives. L'extraction des composés a été réalisée par macération hydroalcoolique avec un rendement de 10,2 %. Le criblage phytochimique a mis en évidence la présence notable de glucides réducteurs, ainsi que de flavonoïdes, de composés phénoliques et de coumarines, tandis que les alcaloïdes, les tanins, les terpénoïdes et les saponosides se sont révélés absents. La teneur en lipides a été déterminée par extraction à l'hexane selon la méthode de Soxhlet, elle est de 5.66 %. Le dosage des glucides a été fait par la méthode de Biuret, la concentration a été estimée à 0,185 mg équivalent glucose/mg d'extrait. La teneur en protéines totales de l'extrait brut a été déterminée par la méthode de Biuret, la concentration a été estimée à 0,08 mg équivalent BSA/mg d'extrait. Ces résultats soulignent l'intérêt thérapeutique potentiel de P. ostreatus, tout en suggérant qu'une optimisation des techniques d'extraction pourrait en améliorer l'efficacité.

Mots clés : Pleurotus ostreatus, champignon comestible, composés bioactifs, extraction hydroalcoolique.

Phytochemical and Biological Investigation of Perralderia coronopifolia Extracts

Sara Boussaha[1,2], Fadila Benayache[1], Samir Benayache[1]

[1] Unité de Recherche : Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques, Université Frères Mentouri, Constantine, Algérie.

[2] Higher National School of Biotechnology Taoufik KHAZNADAR, nouveau Pôle universitaire Ali Mendili, BP. E66, Constantine, 25100, Algeria.

Corresponding author : Boussaha Sara (boussahasarah@yahoo.fr)

Abstract

Aromatic and medicinal plants play a key role in healthcare and various applied fields due to the diversity of bioactive compounds they contain. The present study focuses on the phytochemical characterization and biological evaluation of butanol extracts obtained from the leaves and flowers of Perralderia coronopifolia. HPLC analysis revealed the presence of quercetin in the leaf extract and citric acid in the flower extract. The antioxidant potential of both extracts was assessed using DPPH and ABTS assays, demonstrating significant activity. The ABTS test, in particular, showed a strong antioxidant effect for the butanol leaf extract (IC_{50} = 0.09 ± 0.11 mg/mL) compared to ascorbic acid (IC_{50} = 0.03 ± 0.01 mg/mL). Both extracts were rich in total polyphenols and flavonoids, supporting the observed antioxidant activity. The hemostatic activity evaluation indicated that the butanol extracts from both organs enhance plasma coagulation. Furthermore, anti-inflammatory assays revealed notable activity for the flower extract (IC_{50} = 0.23 ± 0.01 mg/mL) and moderate activity for the leaf extract (IC_{50} = 0.94 ± 1.05 mg/mL) compared to sodium diclofenac (IC_{50} = 0.15 ± 0.01 mg/mL). Overall, Perralderia coronopifolia appears to be a promising source of natural antioxidant, anti-inflammatory, and hemostatic agents, supporting its potential use in pharmaceutical and therapeutic applications.

Keywords: Perralderia coronopifolia, butanol extract, antioxidant activity, anti-inflammatory activity, hemostatic activity.

Bupleurum lancifolium extract as a green corrosion inhibitor for carbon steel in HCl medium

Ilhem Selatnia [1,2], Sirid Remache [3,4], Oday Khamamysa [5], Merzoug Benahmed [6,7]

[1]Laboratory of Analytical Sciences, Material and Environment, LSAME, University of Larbi Ben M'Hidi, Oum El Bouaghi, 04000, Algeria
[2]Laboratory of Electrochemistry of Molecular and Complex Materials (LEMMC), Faculty of Sciences, Department of Chemistry, University Ferhat Abbas Setif-1, DZ-19000, Setif, Algeria.
[3]Laboratory of Natural Resources and Management of Sensitive Environments (LRNAMS) Université Oum-EL-Bouaghi, 04000, Algeria
[4]Scientific and Technical Research Center in Physico-chemical Analysis (CRAPC), BP 384, Zone Industrielle Bou-Ismail RP 42004 Bou-Ismail, Tipaza, Algeria
[5]Biochemistry and Organic Laboratory, Modern University College, Ramallah, Palestine
[6]Laboratory of Bioactive Molecules and Applications, Tebessa University, Route de Constantine, Tebessa 12000, Algeria
[7]Faculty of Exact Sciences & Natural & Life Sciences, Department of Chemistry, Larbi Ben Mhidi University, Algeria

Corresponding author: Selatnia Ilhem (ilhem.selatnia@univ-setif.dz)

Abstract

The use of environmentally friendly corrosion inhibitors for metals and alloys has gained great importance due to their low cost and ecological benefits. In this study, Bupleurum lancifolium extract is introduced as a sustainable corrosion inhibitor for carbon steel in acidic environments. Its inhibition efficiency and adsorption mechanism were explored through electrochemical techniques, and surface characterization. Results indicate that the extract achieves an impressive inhibition efficiency of 97.25% at a concentration of 700 ppm. Overall, this study presents Bupleurum lancifolium extract as a highly effective, green corrosion inhibitor, providing both environmental and scientific value for future inhibitor design and application.

Keywords: Corrosion inhibition, Carbon steel, Adsorption, Bupleurum lancifolium

Comprehensive Profiling of the “Sacred Tree”: Antioxidant Perspectives

Saida SERIDI, **Radia SELAIMIA [b], Roqiya BOUKAHILI, Fatima BOUSAID,**
[*a] Laboratoire de Chimie Physique, Université 08 Mai 45, BP40, Guelma 24000.
[b] Laboratoire d'Analyse Industrielle et Génie des Matériaux. Université 8 mai 1945, Guelma, Algérie
seridi.saida@univ-guelma.dz,
seridisaida77@yahoo.fr

Abstract

Moringa oleifera, a species native to the Himalayan region of India and known as the "tree of life," belongs to the Moringaceae family and is valued for its nutritional, therapeutic, and preventive properties. This study seeks to analyze its chemical composition, particularly focusing on polyphenols and flavonoids, to evaluate its antioxidant and antibacterial potential in vitro.
Extraction was performed through maceration in an 80/20 methanol/water mixture, followed by liquid-liquid extraction using solvents of increasing polarity (petroleum ether, chloroform, ethyl acetate, and n-butanol), achieving yields ranging from 0.7% to 4.6%. The polyphenol content, measured by the Folin-Ciocalteu method, was highest in the butanol extract (4.7 mg/ml gallic acid equivalent). Similarly, the flavonoid concentration, assessed through the $AlCl_3$ colorimetric method with quercetin as a reference, was also highest in the butanol extract (4.32 mg/ml).
Antioxidant activity was tested using DPPH and FRAP assays, with the butanol extract showing the strongest effect (IC50 = 1.988 mg/ml).

Key words: Moringa oleifera, polyphenols, flavonoids, antioxidant activity, DPPH, FRAP.

Study of Phenolic Compounds, antioxidant and Antibacterial activity of Henophyton deserti

Smaali S[1,2], Yousfi A[1], Zaoua F[1], Keziz D. Ed[2], Mesbahi M[1]

[1] Department of Applied Biology, Faculty of Exact Sciences and Natural and Life Sciences, Echahid Echikh Larbi Tebessi University, 12000 Tebessa, Algeria.

[2]Laboratory of toxicology and pathology of ecosystems, Echahid Echikh Larbi Tebessi University, 12002 Tebessa, Algeria;

saoussene.smaali@univ-tebessa.dz

Abstract

The present study aims to evaluate the antibacterial and antioxidant activities of aqueous and methanolic extracts of Henophyton deserti, a medicinal plant traditionally used in the Sahara, in response to the growing issue of antibiotic resistance. Extracts were obtained by maceration in distilled water and a hydro-methanolic mixture, then tested against several bacterial strains using the agar diffusion method, and by determining the minimum inhibitory (MIC) and bactericidal (MBC) concentrations. Extraction yield, total polyphenol content, and antioxidant activity (DPPH assay) were also assessed using the Folin–Ciocalteu method.

Results indicated that the methanolic extract exhibited both a higher extraction yield and stronger antibacterial activity than the aqueous extract, with inhibition zones exceeding 13 mm and MBC/MIC ratios between 1 and 2, reflecting an effective bactericidal effect, particularly against Gram-positive strains. Conversely, the aqueous extract demonstrated notable antioxidant activity compared to the methanolic extract.

These findings suggest that Henophyton deserti represents a promising natural source of antibacterial and antioxidant compounds. Further investigations, particularly in vivo studies, are required to validate its therapeutic potential and to identify the bioactive molecules responsible for these effects.

Keywords: Henophyton deserti, medicinal plant, antibacterial activity, antioxidant, Sahara, Algeria

Study of the Antimicrobial Effect of Tow Medicinal Plants (Comparative Study)

S. Smaali [1,2], F. Zaoua [1], A. Yousfi [1], D. Keziz. L.Rouigui [1], K. Boumaraf [1], I. Boudraa [1], A. Houam [1], [2, M.] Mesbahi [1]

[1] Department of Applied Biology, Faculty of Exact Sciences and Natural and Life Sciences, Echahid Echikh Larbi Tebessi University, 12000 Tebessa, Algeria.

[2]Laboratory of toxicology and pathology of ecosystems, Echahid Echikh Larbi Tebessi University, 12002 Tebessa, Algeria;

saoussene.smaali@univ-tebessa.dz

Abstract

The objective of this study is to evaluate the antifungal activity of methanolic and aqueous extracts of tow medicinal plants; Henophyton deserti and Artemisia herba-alba. The plant material was collected on-site and subjected to traditional extraction protocols using water and methanol.
The evaluation of antimicrobial activity was conducted on pathogenic bacterial, yeast and mold strains using agar diffusion and microdilution tests.
The study results highlighted a generally superior antimicrobial efficacy of the methanolic extracts compared to the aqueous extracts, particularly those from Henophyton deserti, Artemisia herba-alba. Notable variations were observed depending on the type of plant, the solvent used, and the strains examined.
In conclusion, the tested samples, particularly those obtained from methanol, demonstrate promising potential for the design of natural origin antifungal and antibacterial therapies.

Keywords: Henophyton deserti, Artemisia herba-alba, MIC, MFC, naturel alternative.

A Direct and Efficient Synthesis of Glycoconjugated Thioureido-Arylsulfonamides from Unprotected Carbohydrates

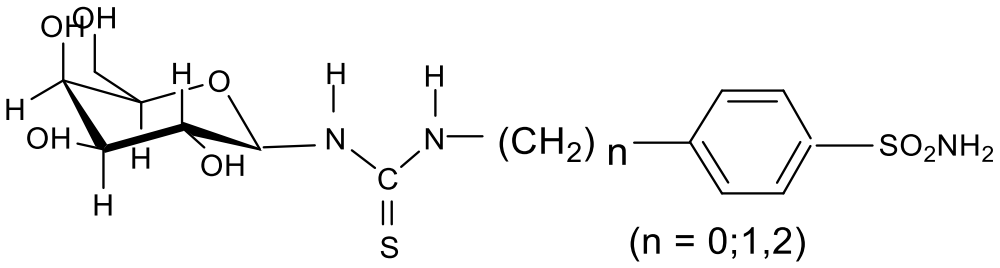
Maamar Stiti [1], Habiba Bouzit [2], Rabah Ksouri [3] and A--G Boudjahem[4]

[1] Department of Material Sciences, Laboratory of Applied Chemistry, University of Guelma, Guelma, Algeria.
[2] Research Centre in Analytical Chemistry and Physics, University of Guelma, Guelma, Algeria.
[3] Department of Process Engineering,Laboratory of Applied Chemistry,University of Guelma, Guelma, Algeria.
[4] Department of Material Sciences, Laboratory of Applied Chemistry, University of Guelma, Guelma, Algeria.
Corresponding author: Stiti Maamar (stiti.maamar@gmail.com)

Abstract

This work focuses on developing efficient and selective inhibitors of carbonic anhydrase IX (CAIX) for the diagnosis and treatment of hypoxic tumors.

A series of three novel thiourea-bridged glycoconjugate benzene sulfonamides (N-(D-xylosyl) thioureido-benzene sulfonamide) was synthesized in short reaction times with easy purification and good yields, by coupling unprotected D-xylosamine with benzene sulfonamide isothiocyanates. The combination of a carbohydrate vector, thiourea linker, and benzene sulfonamide core offers a versatile scaffold for the design of selective and potent CA inhibitors.



Keywords: carbonic anhydrase IX, glycoconjugate, benzene sulfonamide, carbohydrate, thiourea linker, unprotected sugars, xylose.

Ultrasound-Assisted Synthesis and Antimicrobial Evaluation of Functionalized Vanillin Derivative

Takoua Belghit[1], **Abdelkrim Gouasmia** [1]

[1]Laboratory of Organic Materials and Heterochemistry (LOMH), Echahid Cheikh Larbi Tebessi University, Constantine Road, 12002, Tebessa-Algeria.
E-mail: takoua.belghit@univ-tebessa.dz

Abstract

Heterocyclic compounds represent a fundamental class of organic molecules that have attracted considerable interest among organic chemists [1]. Within this group, sulfur-containing heterocycles are particularly notable for their significant bioactivity, both in natural and synthetic molecules.
Vanillin, a well-known oxygenated aromatic compound, exhibits a wide range of biological activities [2–4]. Numerous structural modifications of its heterocyclic core have been explored to enhance its biological properties.
This study focuses on the synthesis, characterization, and electrochemical investigation of a novel vanillin derivative incorporating the 4,5-dimethyl-1,3-dithiol-2-yl moiety. This compound was synthesized through the condensation of vanillin with an alkylated selenone in a trialkylphosphite medium under ultrasonic irradiation.
Various spectroscopic techniques, including infrared (IR) spectroscopy, proton and carbon nuclear magnetic resonance (^{1}H and ^{13}C NMR), mass spectrometry was employed to determine the structural features of the synthesized compound.

The antimicrobial activity of the synthesized functionalized vanillin derivative was tested against some common bacterial pathogens. Interestingly, the compound showed notable inhibition on the growth of P. aeruginosa, E. coli, B. anthracis and C. albicans which suggests that it might serve as an effective antibacterial agent.

Keywords: Vanillin, 1,3-dithiol-2-selenone, Functionalization, Ultrasonic Irradiation, Antimicrobial Evaluation

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Investigation computationnelle du complexe d'inclusion hôte–invité entre la β-cyclodextrine et la 5-fluoro-2-hydroxypyrazine-3-carboxamide

Takoua Belghit[1], Tahar Abbaz[2], Abdelkrim Gouasmia[1]and D. Villemin[3]

1 Laboratory of Organic Materials and Heterochemistry (LOMH), Echahid Cheikh Larbi Tebessi University, Constantine Road, 12002, Tebessa-Algeria.

2 Laboratory of Organic Chemistry and Interdisciplinarity "LCOI", University of Mohamed-Cherif Messaadia, Souk Ahras, 41000, Algeria.

3 Laboratory of Molecular and Thio-Organic Chemistry, UMR CNRS 6507, INC3M, FR 3038, Labex EMC3, ensicaen & University of Caen, Caen 14050, France

E-mail : takoua.belghit@univ-tebessa.dz

Abstract

Le 5-fluoro-2-hydroxypyrazine-3-carboxamide est un composé antiviral reconnu pour sa capacité à inhiber la réplication virale. Dans ce travail, la théorie de la fonctionnelle de la densité (DFT) a été appliquée afin d'étudier le complexe d'inclusion hôte–invité former entre la β-cyclodextrine (β-CD) et le 5-fluoro-2-hydroxypyrazine-3-carboxamide, aussi bien en phase gazeuse qu'en phase aqueuse.

Les calculs quantiques ont permis d'évaluer et d'interpréter les énergies, les paramètres géométriques. Les possibilités d'interactions intermoléculaires entre le 5-fluoro-2-hydroxypyrazine-3-carboxamide et la β-cyclodextrine ont été analysées à l'aide des méthodes NBO (Natural Bond Orbital) et NCI (Non-Covalent Interactions).

Cette étude théorique fournit des informations complémentaires et utiles sur le phénomène de complexation, difficilement accessible par des méthodes expérimentales.

Keywords : 5-fluoro-2-hydroxypyrazine-3-carboxamide/β-cyclodextrine - DFT – NBO - NCI.

Dosage and identification of metformin hydrochloride in an antidiabetic drug «DIABAMINE 1000 mg/Cp» by UV-Visible spectrophotometer

Wassila Yahia [1a*], Ahlam Chiheb [1b], Rahma Achouri [1b] Amel Chalabi [1b]

[1]Chemistry Department, Faculty of Sciences, University of 20 August 1955 - Skikda, P.O. Box 26, El-Hadaiek Road, 21000, Skikda, Alger

[a](MCA) Laboratory of Synthesis and Organic Biocatalysis (LSBO), Organic Synthesis and Medicinal Chemistry Group,
BADJI Mokhtar-Annaba University, Annaba, 23000 Algeria

[b](Doctorant) Laboratoire of Physico-Chimie Des Surfaces Et Interfaces, University 20 August 1955 Skikda, Skikda, Algeria

[*]Corresponding author: Tel./0656631865; E-mail address: w.yahia@univ-skikda.dz

Abstract

The pharmaceutical industry is of great importance and the quality control process of drugs is essential and mandatory for the safety of the product and the consumer simultaneously. In this context, the present study describes the tests to verify the quality of a type 2 antidiabetic drug from the biguanide family: DIABAMINE 1000 mg/Cp. The content uniformity test applied consists of determining the individual contents of metformin hydrochloride by measuring the solutions of DIABAMINE 1000 mg/Cp tablets, using an appropriate analytical method which is the UV-Visible spectrophotometer. For the identification of the active ingredient; the UV-Visible absorption spectra obtained with the solutions of the tablets to be examined can be superimposed on the absorption spectrum of the reference solution (pure metformin hydrochloride) characterized by a maximum absorption at λmax = 233 nm. The dosage of the active ingredient in the tablets is validated taking into account the Beer-Lambert law and the dosage protocol. The content of metformin hydrochloride is between 85% and 99%, indicating that the active ingredient content conforms to the standard of the European Pharmacopoeia.

Keywords: Spectrophotometric analysis, DIABAMINE 1000mg/Cp, metformin hydrochloride.

Biological Treatment of Wastewater for Pollutant Removal Using Agaricus bisporus mushroom

Yehya Bouraghda [12], Abderrahim Boutemedjet [3]

[1] Department of Process Engineering, University of 8 Mai 1945, Guelma, Algeria
[2] Department of Process Engineering, Laboratory of Organic Synthesis, Modeling, and Optimization of Chemical Processes, University of Badji Mokhtar, Annaba, Algeria
[3] Departement of Process Engineering, Laboratory of Physics for Matter and Radiation, University of Souk Ahras, Souk Ahras, Algeria
Corresponding author: Bouraghda Yehya (bouraghda.yehya@univ-guelma.dz /yehya.boureghda@univ-annaba.org)

Abstract

The growing amount of water resources pollution by industrial effluents and heavy metals needs the creation of affordable and sustainable treatment options. This paper investigates the edible mushroom Agaricus bisporus as a natural biosorbent for wastewater purification. Fresh and dried mushroom biomass was used to take away heavy metals and organic pollutants on simulated and real wastewater samples respectively obtained in the local industries. The biosorption experiments were performed at controlled conditions in batch mode, to determine the effect of pH, contact time, initial concentration of pollutants and biomass dosage on the removal efficiency. UV-Vis spectrophotometry was used to determine the metal uptake and reduction of organic matter in the treated water and the mushroom biomass. The highest removal efficiencies were recorded in/near-neutral pH and moderate contact time where A. bisporus showed the highest affinity to lead, copper, and chromium ions with removal efficiencies of over 70 percent. Fourier-transform infrared (FTIR) analysis showed the presence of functional groups that included hydroxyl, carboxyl, and amine residues on the mushroom surface that were the binding sites of the metal. The above results demonstrate the promise of Agaricus bisporus biomass-a low-cost and food industry by-product that is inexpensive and renewable-as an effective and environmentally friendly wastewater treatment material. The biological method offers a potential solution to sustainable water treatment and is relevant to the growth of circular bio-based engineering with water treatment.

Keywords: Agaricus bisporus; Biosorption; Wastewater treatment; Heavy metals; Sustainable technology; Circular bioeconomy.

Natural Products Recovery of Tomato Industrial Residues by using Eco-Friendly Extraction Methods

Yehya Bouraghda [12], Abderrahim Boutemedjet [3]

[1] Department of Process Engineering, University of 8 Mai 1945, Guelma, Algeria
[2] Department of Process Engineering, Laboratory of Organic Synthesis, Modeling, and Optimization of Chemical Processes, University of Badji Mokhtar, Annaba, Algeria
[3]Departement of Process Engineering, Laboratory of Physics for Matter and Radiation, University of Souk Ahras, Souk Ahras, Algeria
Corresponding author: Bouraghda Yehya (bouraghda.yehya@univ-guelma.dz /yehya.boureghda@univ-annaba.org)

Abstract

By-products of tomato processing industry in Guelma, Algeria, include peels, seeds, and pulp remnants that are usually disposed of even though they contain a lot of valuable bioactive compounds. This research seeks to transform these agro-industrial wastes into valuable resources through sustainable valorization by extracting natural antioxidants and pigments using environmentally-friendly and sustainable procedures. In order to isolate lycopene, b-carotene and phenolic compounds in tomato residues collected in local canning factories, ethanol-water mixes and ultrasound-assisted extraction technique were used. UV-V analyses were used to find out the purity of extracts. The findings also revealed that green methods of extraction increase the recovery efficiency greatly with little consumption of solvents and low environmental effects. The recovered compounds had a good antioxidant potential and this reveals their potential application as natural colorants and preservatives in food, cosmetic and pharmaceutical preparations. This project is part of the regional circular economy because it turns tomato waste into high-value natural products with the help of sustainable process engineering.

Keywords: Waste tomatoes, lycopene, green extraction, antioxidants, circular economy, Guelma, Algeria

Phytochemical composition and biological activities of Citrus aurantium methanolic leaf extract

Zineb Rania Belaifa[1], Nermine Bouhallit[2]

[1]Department of Biochemistry, University of badji mokhtar, Annaba, Algeria
[2]Department of Pharmacy, University of badji mokhtar, Annaba, Algeria
Corresponding author: Zineb Rania Belaifa (belaifarania07@gmail.com)

Abstract

Citrus aurantium L., commonly known as bitter orange, is a medicinal plant widely studied for its diverse bioactive compounds and therapeutic properties. This study aims to explore the phytochemical profile and biological activities of Citrus aurantium leaf methanolic extract.

Phytochemical screening of the methanolic extract revealed the presence of phenolic compounds, flavonoids, and saponins, confirming a rich diversity of secondary metabolites. Quantitative analyses demonstrated high total phenolic content (219.56 mg GAE/g) and considerable flavonoid content (77.33 ± 14.16 mg QE/g), highlighting the plant's potential as a valuable source of natural bioactive compounds.

The antioxidant activity, evaluated using the DPPH radical scavenging assay, showed moderate potency with an IC_{50} value of 0.2998 mg/mL compared to ascorbic acid (IC_{50} = 0.056 mg/mL). In contrast, the extract exhibited strong anti-inflammatory potential in the ovalbumin denaturation assay, with an IC_{50} of 0.1521 mg/mL—surpassing the reference drug diclofenac (IC_{50} = 0.9 mg/mL). However, the methanolic extract showed no antibacterial effect against Escherichia coli, Salmonella spp., Pseudomonas aeruginosa, or Staphylococcus aureus.

Keywords: Citrus aurantium, methanolic extract, phenolic compounds, flavonoids, biological activities.

Electrochemical Study of Mg^{2+}–Lomustine and Zn^{2+}–Lomustine Metal Complexes: Characterization by Cyclic Voltammetry and Anticancer Implications

Hassina Fisli [1], Mohamed Lyamine Chelaghmia [2]

[1] Material sciences department, Laboratory of Applied Chemistry (LCA), 8 mai 1945 Guelma University, Guelma, Algeria
[2] Process Engineering Department, Materials analysis and engineering laboratory (LAIGM), 8 mai 1945 Guelma University, Guelma, Algeria
Corresponding author: Fisli Hassina (fisli.hassina@univ-guelma.dz)

Abstract

Lomustine (CCNU) is a nitrosourea-based alkylating anticancer agent widely used in the treatment of brain tumors, malignant melanoma, and certain types of lung cancer. Its lipophilic nature allows it to cross the blood–brain barrier, making it particularly effective against central nervous system malignancies. The drug exerts its cytotoxic effect mainly through DNA alkylation, causing strand breaks and inhibition of cellular replication. Previous studies have shown that metal–drug interactions can significantly alter the redox behavior, stability, and bioactivity of several nitrosourea derivatives, suggesting that complexation with biologically essential metal ions could modulate their therapeutic potential. A comparative electrochemical study of Mg^{2+}–lomustine and Zn^{2+}–lomustine complexes was conducted. Cyclic voltammetry, supported by potentiometric measurements, was employed to elucidate the metal–ligand interactions and determine key electrochemical parameters. The findings suggest that Zn^{2+} enhances the stability and electrochemical activity of lomustine. These findings highlight the crucial role of the metal ion in modulating the electrochemical and potentially the pharmacological behavior of lomustine. Future perspectives include extending this study to other transition metals and correlating electrochemical data with kinetic, spectroscopic, and biological analyses. Such an integrated approach could contribute to the rational design of new metal-based lomustine derivatives with improved stability, selectivity, and anticancer efficiency.

Keywords: Anticancer agents, Lomustine, Metal complexes, Electrochemistry, Coordination chemistry

Phytochemcal analysis, Molecular Docking study of Compounds Isolated from Senna alexandrina aqueous exract

Hayette Ayed[1,2], Maroua Belkheit[1], Awatif Boumaaza[1], Rabeh Zebsa[2,3], Hamdiken Malika[1]and Amira Chorfi [1]

[1]Faculty of natural and life sciences, Earth and the Universe, department of biology, university 8Mai 1945 Guelma
[2] Labortoire Biologie, Eau et Environnement LBEE.
[3] Faculty of natural and life sciences, Earth and the Universe, department of Ecology and environment, university 8Mai 1945 Guelma.

Abstract

Senna alexandrina has been traditionally employed for its laxative properties; however, its potential antibacterial and gastroprotective activities remain insufficiently investigated. This study aimed to characterize the phytochemical composition and the molecular docking for the most abandant. molecules. Phytochemical profiling was conducted using LC-MS QTOF and FTIR techniques on aqueous extract of the plant In molecular docking was performed to evaluate the interactions of major phytoconstituents with bacterial RNA polymerase and gastric H^+/K^+-ATPase. several predominant compounds were identified. These included phenolic acids such as gallic acid and citric/isocitric acid, and flavonoid derivatives, notably flavonoid glucosides and pentahydroxyflavone O-glucoside. Additionally, the presence of sennosides A and B, which are recognized for their potent laxative effects, was confirmed., The FTIR spectrum of the aqueous extract showed several distinct absorption bands. The broad band between 3600 and 3200 cm^{-1}. Docking studies indicated strong binding affinities of key phytochemicals with both bacterial and gastric targets. In conclusion, the aqueous extract of Senna alexandrina demonstrates promising antibacterial and gastroprotective activities, likely attributable to its rich polyphenolic composition. These results support its traditional medicinal use and highlight its potential as a source of bioactive therapeutic agents.

Key words, molecular docking, FTIR, antibacterial

Synthesis and antibacterial activity of some new derivatives imidazole

Zama Sana[1*], benosmane ali[2,3] ,[1]Hamimed Souad[1], Zater Hanène[1,4]

e-mail: sanazama98@yahoo.fr

[1]1Laboratoire des Sciences Analytiques Matériaux et Environnement. (SAME), Université d'Oum El Bouaghi « Larbi Ben M'Hidi», PB 358 route de Constantine, PB 358 route de Constantine, Oum el Bouaghi 04000, Algeria.
2 Department of matter sciences, University of Oum EL-Bouaghi, Oum El Bouaghi 04000, Algeria
3 Research Unit of Environmental Chemistry and Molecular Structural (CHEMS), University of Constantine 1 (Mentouri), 25000 Constantine, Algeria
[4]Unité de recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques (VARENBIOMOL), Département de Chimie, Faculté des Sciences Exactes, Université FrèresMentouri Constantine 1, Route d'Aïn El Bey, 25000, Constantine, Algeria

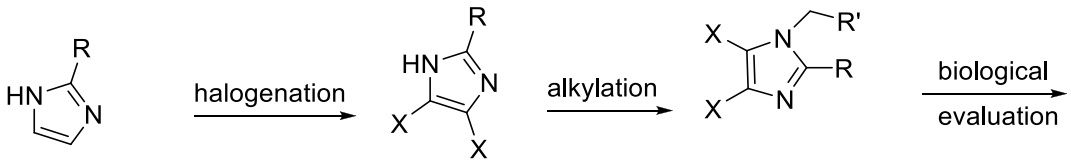
Abstract

The widespread use of antimicrobial agents has resulted in the development of resistance to these drugs by pathogenic microorganisms, causing an increase in morbidity and mortality.

One of the strategies to overcome this problem is to identify new drugs with a new molecular target. The imidazole nucleus is an important building block in drug discovery.[1]Recently imidazole and imidazolium derivatives have been the subject of extensive study for their therapeutic potential as effective antimicrobial agents.[2]Indeed, the N-substituted imidazole shows a great variety of biological activity in pharmacology, such as antiparasitic, antifungal,[3]and antimicrobial.[4]

In other hand, some halogenoimidazoles have been used in therapeutic as antibacterial, antidiabetic, antihypertensiveand in agriculture sector such as herbicides, fungicides, pesticides, etc.[5]

In the present work, a variety of some new functionalized halogenoimidazoles compounds were prepared (variations on C_2, C_4 and C_5) by successive functionalization of imidazole and their antimicrobial activity towards positive and gram-negative bacteria was studied. The structure elucidation of some prepared compounds was performed by IR, NMR. The general synthetic scheme is described above:



Keywords: N-Substituted imidazole, haloimidazoles, antibacterialactivity.

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Assessment of the Antioxidant and Antimicrobial Potential of Marian thistle L

ALIOUCHE Lamia [1]*& ZATER Hanène [1,2]

[1]Unité de recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques (VARENBIOMOL), Département de Chimie, Faculté des Sciences Exactes, Université Frères Mentouri Constantine 1, 25000 Constantine, Algeria.
[2]Département des sciences de la matière, Faculté des sciences exactes et sciences de la nature et de la vie, Université Larbi Ben M'Hidi, Cité du 1er Novembre 1954, B.P. 358 Route de Constantine, 04000 Oum El Bouaghi, Algeria.
Email of communicant:aliouche@yahoo.com
E-mail professionnelle : aliouche.lamia@umc.edu.dz

Abstract:

Marian thistle L (Asteraceae) is a well-known medicinal plant traditionally used for liver disorders. Despite extensive global studies, it remains poorly investigated in Algeria. This work aims to assess its phytochemical composition and biological activities, focusing on its antioxidant and antimicrobial potentials.

The contents of total polyphenols and flavonoids were quantified using colorimetric methods; Folin-Ciocalteu and aluminum trichloride, respectively. The findings revealed that the n-butanol extract exhibited the highest concentrations of both polyphenols and flavonoids.

The antioxidant potential of the extracts was evaluated using four complementary assays: DPPH, ABTS, FRAP and phenanthroline. The results showed that the ethyl acetate and n-butanol extracts possessed moderate antioxidant activity when compared with the reference standards.

The antifungal and antibacterial activities of the extracts were also tested against two bacterial strains; Escherichia coli and Staphylococcus aureus. The results revealed a marked bacteriostatic effect, particularly for the ethyl acetate and n-butanol extracts, which displayed strong inhibitory zones against both microorganisms, indicating that the bioactive compounds contained in these extracts possess significant antibacterial properties.

Keywords : Asteraceae, Marian thistle L, polyphénols dosage, antioxydant activity, antimicrobial potential

Application Of the Design of Experiments Methodology to The Improvement of Essential Oil Extraction

Belleili Mehdi[1,2], Hadef Youcef[1,2].

1 Analytical Chemistry Laboratory, Faculty of Medicine, Badji Mokhtar University, Annaba
2 Laboratory for the Development and Control of Hospital Pharmaceutical Preparations, Faculty of Medicine, Badji Mokhtar University, Annaba
Corresponding author: Belleili Mehdi (mmbelleili@yahoo.fr)

Abstract

Rosemary, Rosmarinus officinalis L., is a medicinal herb widely used throughout the world. It is undoubtedly one of the most popular plants in Algeria. Rosemary contains an essential oil to which it owes its valuable properties.

The objective of this work is to model and optimize the hydrodistillation process of Rosmarinus officinalis L. using the design of experiments methodology.

The Rosmarinus officinalis L. was harvested from the garden of the Faculty of Medicine in Annaba during the month of January. The apparatus used for hydrodistillation was a Clevenger type. The essential oil yield, according to the postulated and validated mathematical model, depends on the following linear terms: hydrodistillation time, drying time, and heating temperature, respectively. For this plant, a hydrodistillation time of 150 minutes, a heating temperature above 220°C, a water-to-plant-material ratio greater than 1.7 (x 100 g/1000 mL), and a drying time of 6 days are the optimal experimental conditions for maximizing the yield to 2.1%, compared to the usual 1.4%. These results can serve as a basis for extrapolating the optimization of experimental conditions for essential oil extraction using pilot or industrial processes. Therefore, they could be of significant economic interest.

Keywords: Yield, Extraction, Essential oil, Experimental design, Optimization

Antioxidant Activity of Ephydra Species

Berkane Aya[1]*, Terfassi Siham[2], Laraba Meriem[3], Zouioueche Kaouther[3], Erenler Ramazan[4], Benayache Fadila[5], Benayache Samirm[5], Zama Djamila[6]

1. Department of Biochemistry and Cellular and Molecular Biology, University of Constantine 1aya.berkane@doc.umc.edu.dz

2.Department of exact sciences, University of Constantine 1,Laboratory of Valorization of Natural Resources, Bioactive Molecules, and Physico-Chemical and Biological Analysis (VARENBIOMOL), Chaabet Ersas Campus, 25000 Constantine, Algeria.* siham.terfassi@.umc.edu.dz
2.3. Department of Animal Biology, Faculty of Natural and Life Sciences,University of Constantine 1, Route d'Aïn El Bey, 25000 Constantine, *Algeria.m_laraba@yahoo.com *kaouther.zouioueche@doc.umc.edu.dz
4.Research Laboratory and Application Center (ALUM), Foundation of the Faculty of Health Sciences,Department of Nutrition and Dietetics, Iğdır University, Iğdır, 76000, Turkey, *alum@igdir.edu.tr
5.Department of exact sciences, University of Constantine 1,Laboratory of Valorization of Natural Resources, Bioactive Molecules, and Physico-Chemical and Biological Analysis (VARENBIOMOL), Chaabet Ersas Campus, 25000 Constantine, *fadila.benayache@umc.edu.dz *benayache.samir@umc.edu.dz
6.Department of Animal Biology, Faculty of Natural and Life Sciences,University of Constantine 1,Laboratory of Valorization of Natural Resources, Bioactive Molecules, and Physico-Chemical and Biological Analysis (VARENBIOMOL), Chaabet Ersas Campus, 25000 Constantine, Algeria, *zamadjamila@yahoo.fr
Email*: aya.berkane@doc.umc.edu.dz

Abstract – The genus Ephydra, comprising several extant species, is native to arid and semi-arid regions and has garnered significant scientific interest due to its potential bioactive properties. This study evaluated the antioxidant activity of ethyl acetate (EAE), n-butanol (BEE), chloroformic (CE), and petroleum ether (PEE) extracts from an Ephydra species using the in vitro DPPH radical scavenging assay. The results demonstrated that all extracts exhibit varying degrees of antioxidant activity, with (CE) and (EAE) showing the highest potential, likely due to their richness in polyphenols. The findings suggest that Ephydra species may serve as a valuable natural source of antioxidants with potential applications in pharmaceutical and nutraceutical fields.

Keywords: Ephydra, DPPH assay, antioxidant activity.

Nouveaux Sulfahydantoines Modifiées Issues de la Glycine via une Réaction D'aldolisation : Synthèse, Structure et Aspect Stéréochimique

Djamel Bouchouk[1], **Fatma Zohra Souha Soukehal, Tahar Abbaz**

[1]Laboratoire de Chimie Organique et d'Interdisciplinarité, Université Mohamed Cherif Messaadia de Souk Ahras, Algérie.

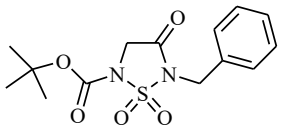
Djamel Bouchouk, E-mail: d.bouchouk@univ-soukahras.dz

Résumé

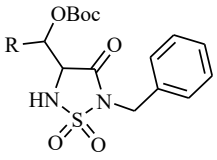
Les sulfahydantoïnes de type (1,1- dioxydes -3- oxo- 1, 2, 5-thiadiazolidines), sont décrites sur le plan pharmacologique et chimique comme des composés potentiellement inhibiteurs de protéases virales, et aussi comme aglycones entrant dans la structure de pseudonucléosides décrits dans la littérature comme des antiviraux et/ou antitumoraux. Dans des travaux antérieurs, nous avons décrits la synthèse de plusieurs types de sulfahydantoïnes.

Le travail présenté dans cet exposé est consacré à la mise au point d'une nouvelle séquence réactionnel aisée et presque directe qui a conduit à la préparation de la sulfahydantoïne (I) N-protégée par deux groupement protecteurs orthogonaux (Boc et Bn), celle-ci est utilisée comme précurseur pour explorer la réaction d'aldolisation dans la perspective de créer une liaison C-C en position 4 de l'hétérocycle. La méthode de synthèse que nous avons adoptée consistera à faire réagir un équivalent de l'énolate de la glycine issue de la sulfahydantoïne (I) activée avec une série d'aldéhydes, en présence d'une base (DBU) dans le DCM anhydre. Cette condensation et stéréosélective, elle nous a permis d'aboutir à de nouvelles hétérocycles azotés à cinq chainons (II), (III), (IV), (V) avec une diastéréoisomérie **syn** majoritaire.

Les structures présentées ci-dessous sont parfaitement élucidées par les méthodes Spectroscopiques usuelles.



(I)



(II) R = Et

(III) R = i- Pr

(IV) R = cyclohexyle

(V) R = Ph

Mots clés : Sulfahydantoine, Aldolisation, diastéréosélectivité.

Dosage of metals in some Algerian plant species

Hamimed Souad [1], Zama Sana [1], Zater Hanène [1], Chebout Abderrezzeq [2] and Bekhouche Rahal [1]

[1] Department of Material Sciences, Faculty of Exact Sciences and Natural and Life Sciences, University of Oum El Bouaghi, city of November 1, 1954, B.P.358 Route de Constantine, 04000 Oum El Bouaghi, Algeria.
[2] Department of Applied Sciences. University of Tebessa. Tebessa. Algeria.

Corresponding author: hamimed.souad@univ-oeb.dz

Abstract

The transfer of metallic elements to plants has been widely studied, some elements being trace elements for living organisms [1]. However, at high concentrations, they all become toxic. In plants, this toxicity is due to several reasons [2-3]. The main objective of this work is to quantify metals in plant species commonly used in Algerian medicine (Artemisia herba-alba (ARH), Marrube vulgaris (MAV), Rosmarinus officinalis L. (ROO), and Thymus vulgaris L. (THV). In this context, the present study first aims to determine the physicochemical parameters such as pH, electrical conductivity (three modes of extraction), and organic matter (plant powder). Secondly, the concentrations of metals (Ca, Na, Ba and Li) are estimated by mineralizing the plant powder and measuring the metals using a flame photometer. The results indicated that the lowest pH (6.4 ± 0.07) was recorded in the hot aqueous extract of ARH (metal solubility is higher compared to other extracts), the highest electrical conductivity (0.23ms/cm) was recorded in the hot aqueous extract of THV, while the lowest percentage of organic matter was recorded in the leaf powder of THV (18.71%). Calcium is one of the elements whose contents are the highest in plant tissues; our results show a relatively high rate in MAV (234.323 ppm). The sodium concentration varies widely among the three different plant species, with MAV showing the minimum concentration (5.293 ppm).The barium showing the minimum concentrations in all plants, with a concentration not exceeding 12.397 ppm. Some concentrations are comparable (case of lithium), with a maximum concentration recorded at MAV (142.844 ppm). The measured parameters were also positively correlated with the information obtained from the solid UV spectra of the plants. All the obtained results allow estimating the metal profile in the studied plant species.

Keywords: metallic elements, flame photometer, pH, electrical conductivity.

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Phytochemical Study and Structural Characterization of Secondary Metabolites from the Aerial Parts of an Endemic Steppe Species from Algeria

ZATER Hanène [1,2*], ALIOUCHE Lamia[1], HAMIMED Souad[2], ZAMA Sana[2]

[1]Department of Chemistry, Research Unit for the Valorization of Natural Resources, Bioactive Molecules, and Physicochemical and Biological Analyses (VARENBIOMOL), Frères Mentouri University of Constantine-1, Faculty of Exact Sciences, Aïn El Bey Road, 25000, Constantine, Algeria.
[2]Department of Matter Science, Faculty of Exact Sciences and Natural and Life Sciences, University of Oum El Bouaghi « Larbi Ben M'Hidi », P.O. Box 358 Constantine Road, Oum el Bouaghi 04000, Algeria.
Corresponding author: h.zater@yahoo.fr; zater.hanene@univ-oeb.dz

Abstract

Due to its diverse geography and ecology, Algeria hosts a remarkably rich flora, including numerous endemic species that remain poorly investigated from a chemical standpoint. As part of an ongoing effort to valorize this biodiversity, the present study focuses on a steppe endemic species belonging to the genus Centaurea (Asteraceae), known for the structural diversity and biological potential of its secondary metabolites. The aerial parts of the plant were extracted by maceration using a hydro-methanolic solvent (80 %), followed by successive fractionation with solvents of increasing polarity. The work focused on the ethyl acetate extract, selected for its high phenolic content. Preliminary phytochemical screening, performed by thin-layer chromatography following the method of Wagner and Bladt and complemented by colorimetric assays, revealed the presence of flavonoids, terpenoids, anthraquinones, and traces of alkaloids. Chromatographic purification steps led to the isolation of a pure secondary metabolite. Its structure was elucidated based on spectroscopic analyses, including HR-ESIMS, HR-EIMS, UV, and 1D/2D NMR (^{1}H, ^{13}C, COSY, ROESY, HSQC, HMBC). Comparison of the obtained spectral data with those reported in the literature allowed for structural identification of the compound. These findings highlight the metabolic richness of this steppe species and provide valuable insight into the chemical composition and scientific valorization of Algeria's endemic flora.

Keywords: Secondary metabolites; ethyl acetate extract; phytochemistry; NMR spectroscopy; mass spectrometry; Algerian endemic flora.

Etude D'une Nouvelle Voie D'accés aux bases de Mannich 'PEG600'

Zetchi Amel[1], Mennana Imen[2], Nemouchi Sara[3], Boumoud Taoues[4]

[1] Département de chimie, Laboratoire de synthèse des molécules bioactives SYMBIO., université Mentouri de Constantine1, Constantine, Algérie.

[2] Département de chimie, Laboratoire de synthèse des molécules bioactives SYMBIO., université Mentouri de Constantine1, Constantine, Algérie.

[3] Département de chimie, Laboratoire de synthèse des molécules bioactives SYMBIO., université Mentouri de Constantine1, Constantine, Algérie.

[4] Département de chimie, Laboratoire de synthèse des molécules bioactives SYMBIO., université Mentouri de Constantine1, Constantine, Algérie.

Corresponding author: Zetchi Amel (melitazetchi@gmail.com)

Abstract

La synthèse organique dans le cadre de la chimie organique moderne se focalise sur les problématiques d'économie (étapes, atomes, énergie). Les réactions à composants multiples (RCMs), visant à synthétiser des produits hautement fonctionnalisés en une unique opération chimique, s'inscrivent précisément dans ce contexte. Par conséquent, ces réactions connaissent aujourd'hui un intérêt considérable tant dans le secteur industriel qu'académique. L'efficacité d'une synthèse organique dépend essentiellement du catalyseur qui focalise le plus de chercheurs, car de là en dépendent l'économie en temps et en énergie, cela nous a exhortés à mener une étude de la réaction de Mannich, une des réactions à composants multiples les plus importantes vue l'utilité de ses produits synthétisés 'β-aminocétones' dans notre quotidien tels que la Nisoxetine antidépresseur et le tolmetin…. Un criblage catalytique nous a orientés sur la détermination d'un nouveau catalyseur dont les essais préliminaires se sont vus très concluants. La généralisation de la voie, après optimisation avec les trois librairies des réactifs, a généré une chimiothèque de bases de Mannich avec de très bons rendements.

Keywords : RCMs, réaction de Mannich, β-aminocétones, criblage, PEG600.

Integrated Chemical Profiling and Bioactivity Assessment of Opuntia ficus-indica Roots: A Novel Source of Antioxidant and Antibacterial Metabolites

Elias Benramdane[1], Nawal Makhloufi[1], Abderezak Tamendjari[1], Cassamo U. Mussagy[2]

[1]Laboratoire de Biochimie Appliquée, Faculté des Sciences de la Nature et de la Vie, Université de Bejaia, Bejaia 06000, Algeria.
[2]Laboratorio de Desarrollo de Bioprocesos Sostenibles (Labisost), Escuela de Agronomía, Facultad de Ciencias Agronómicas y de los Alimentos, Pontificia Universidad Católica de Valparaíso, Casilla 4-D, Quillota 2260000, Chile.

Abstract

This study provides a comprehensive chemical and bioactivity characterization of Opuntia ficus-indica roots from Algeria, highlighting their potential as a sustainable source of bioactive metabolites. Advanced chromatographic and spectrometric techniques were employed to elucidate both phenolic and lipophilic fractions. UHPLC-DAD-ESI-MS/MS analysis identified 26 phenolic compounds—among them piscidic acid, epicatechin-3-O-gallate, and isovitexin— several reported for the first time in this organ. The green and red varieties displayed the highest total phenolic contents (up to 147.8 mg/g extract) and exhibited remarkable antioxidant activity (ABTS IC_{50} = 29 µg/mL; hydroxyl radical inhibition >90%), supported by a high Relative Antioxidant Capacity Index. Dichloromethane extraction afforded up to 5.8 g/kg dw of lipophilic compounds, and GC-MS profiling revealed 55 constituents dominated by β-sitosterol and essential fatty acids such as linoleic and linolenic acids. These extracts showed significant antibacterial activity, with inhibition zones of 19–23 mm against Staphylococcus aureus and MRSA, and MIC values up to 950 µg/mL for Pseudomonas aeruginosa. Incorporation of the antioxidant-rich extracts into handmade soap formulations demonstrated stable radical scavenging properties, validating their applicability in cosmetic chemistry. Overall, this integrative chemical investigation highlights the cactus root as an underexplored matrix combining rich phytochemical diversity with strong biological activity, offering new perspectives for the valorization of agricultural residues in green chemistry, pharmaceuticals, and sustainable product development.

Keywords: Opuntia ficus-indica, phytochemistry, UHPLC-MS/MS, GC-MS; phenolics, sterols, sustainable chemistry.

Contribution à l'étude botanique et phytochimique de deux plantes médicinales du nord est algérien à propriétés antibactériennes Salvia officinalis L. et Lavandula stoechas L.

SAÏDI OUIDED.[1], Farhi Chaima[2], Bouderbala Maissa[3], Maghlaoui Chaima[3], Derradji L[4], Djahoudi A. [5], Hadef Y.[6]

1- Maître de conférences hospitalo-universitaire classe A en pharmacognosie, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.

2- Résidente en pharmacognosie ,faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.

3- Pharmacienne, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.

4- Professeur hospitalo-universitaire et chef de service en pharmacognosie, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.

5- Professeur en microbiologie, Faculté des sciences, Université Badji Mokhtar-Annaba.

6- Professeur hospitalo-universitaire et chef de service en Chimie analytique, Faculté de médecine université Badji Mokhtar-Annaba.

E Mail :widpharm@yahoo.fr

Résumé

La sauge et la lavande sont deux plantes médicinales appartenant à la famille des Lamiaceae très répondues dans le pourtour méditerranéen et qui fournissent des substances intéressantes par leurs divers pouvoirs thérapeutiques ;parmi ces pouvoir on a le pouvoir antibactérien que nous avons évalué au cours de notre étude.

L'objectif visé par cette étude, est de contribuer à la recherche d'un traitement d'appoint aux traitements chimiques, ce qui permet de réduire certains effets indésirables engendrés par ces derniers, de minimiser les phénomènes de résistance aux antibiotiques et de conférer un bénéfice santé favorable.

El effet, nous avons dans un premier temps, procédé à l'identification botanique complète des espèces deLavandula stoechas L. et de salvia officinalis L., et ceci par une description détaillée des caractéristiques macroscopiques ainsi qu'une diagnose de la coupe transversale et la poudre ce qui nous a permis de confirmer la présence des différents constituants caractéristiques de la famille des Lamiaceae.

Le screening phytochimique fût un moyen simple et efficace pour identifier les composés chimiques contenus dans les feuilles de la lavande stéchade et de la sauge officinale.

Ensuite, nous avons effectué l'extraction des huiles essentielles des parties aériennes de Lavandula stoechas L. et de salvia officinalis L. Ces extractions nous ont fourni un rendement en huile essentielle assez faible que ce soit pour la lavande stéchade ou la sauge officinale.

Les propriétés organoleptiques des huiles essentielles de lavandula stoechas L. et salvia officinalis L. sont semblables à celles rapportées dans la littérature

Une analyse chimique des constituants organiques des huiles essentielles extraites, par chromatographie sur couche mince a été réalisée.

Enfin, l'évaluation de l'activité antibactérienne a été testé sur vingt-deux souches bactériennes. Elle a permis de démontrer une variabilité plus ou moins importante en ce qui concerne la sensibilité des souches testées ; certaines sont fortement sensible à l'action des huiles essentielles comme l'Actineto bacterbaumanii tandis que d'autres présentent une résistante totale tel que le pseudomonas aeruginosa

Ce travail de thèse de fin d'étude n'est qu'une tentative de participation à des travaux de recherches scientifiques dont l'objectif principal était la valorisation de la flore Algérienne et contribution à la mise au point de nouveaux principes bioactifs naturels plus efficace et moins nocifs

Mots clés: Lavendula stoechas L; Salvia officinalis L;activité antibactérienne ; huile essentielle

Contribution à l'étude histo-anatomique et étude physicochimique d'une plante médicinales du littoral Algérien: Eucalyptus spp. »

SAÏDI OUIDED.[1], Filali Meriem[2], Niss Mohamed[3], Faarour[3], Derradji L[4], Hadef Y.[6]
Institution: 1- Maître de conférences hospitalo-universitaire classe A en pharmacognosie, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.
2- Assistante en pharmacognosie, CHU Annaba.
3- Pharmacien, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.
4- Professeur hospitalo-universitaire et chef de service en pharmacognosie, faculté de médecine, Université Badji mokhtar-Annaba / CHU Annaba.
5-Professeur hospitalo-universitaire et chef de service en Chimie analytique, Faculté de médecine université Badji Mokhtar-Annaba.
E Mail: widpharm@yahoo.fr

Résumé
Le littoral algérien, et par sa situation géographique particulière est caractérisé par la richesse de sa flore médicinale qui comprend des centaines d'espèces végétales dont l'Eucalyptus spp. qui fait l'objet de notre étude. Le but de notre travail consiste à identifier les caractères histo-anatomiques et la composition chimique, et étudier l'activité antibactérienne des huiles essentielles d'Eucalyptus globulus L et Eucalyptus camaldulensis D récoltées d'Annaba, El-Tarf et Skikda. Après avoir bien identifier la coupe et la poudre des feuilles de notre plante, l'extraction des huiles essentielles par hydrodistillation donne un rendement moyen de 3,4 ml / 100g de feuilles. Pour l'étude physico-chimique, le screening phytochimique détermine la contenance des feuilles en composés chimiques et la chromatographie sur couche mince confirme la présence du terpinéol dans les huiles essentielles des deux espèces. Pour évaluer l'activité antibactérienne de ces essences, un antibiogramme exprime l'inhibition de croissance d'Escherichia coli et Staphylococcus aureus par l'Eucalyptus, ce qui justifie ses emplois dans le traitement de certaines maladies infectieuse, particulièrement les infections respiratoires et digestifs. Mots clés : Plante médicinale, littoral algérien, Eucalyptus spp., hydrodistillation, huile essentielle, terpinéol, activité antibactérienne.

Mechanism and Selectivity of the pdr-type [3+2] Cycloaddition Reaction Between a Chiral Azomethine Ylide and β-Nitrostyrene

Lylia NASRI[1,2], Loubna Oumama[4], Leila Barama[1,3], Abdelmalek Khorief Nacereddine[2].

[1] National Higher School of Technology and Engineering ,23005,Annaba, Algeria
[2] Laboratory of Physical Chemistry and Biology of Materials, Department of Physics and Chemistry, Higher Normal School of Technological Education of Skikda, Azzaba 21300, Skikda, Algeria
[3] Laboratory of Organic Synthesis and Biocatalysis, Badji Mokhtar University, Annaba 23005, Algeria
[4] Applied Biochemistry Laboratory, University of Ferhat Abbas Setif-1 19000, Algeria
l.nasri@ensti-annaba.dz

Abstract

This theoretical study analyses the molecular mechanism and selectivity of the [3+2] cycloaddition (32CA) reaction between a chiral azomethine ylide (AY) and β-nitrostyrene (NS 7), using Molecular Electron Density Theory (MEDT) and DFT methods **[1]**. The Electron Localization Function (ELF) analysis reveals that the AY possesses a pseudodiradical electronic structure (pdr-type). Conceptual DFT reactivity indices classify the AY as a strong nucleophile and NS as a strong electrophile **[2]**, indicating a polar process, while Parr functions correctly predict the high meta regioselectivity (C1-C5 interaction). The study, covering both the experimental reactant (AY 11a) and a simplified model (AY 11b), confirms the reaction has a low activation enthalpy (4.1 kcal/mol for 11a). It is completely meta regioselective and endo stereoselective, in agreement with experimental results **[3]**. The Molecular Electrostatic Potential (MEP) analysis explains the endo stereoselectivity through favourable electrostatic interactions between the AY hydrogens and the nitro group of NS in the transition state. Finally, the ELF analysis of the bond formation process confirms a non-concerted, two-stage one-step mechanism **[4]**.

Keywords: Azomethine, pyrrolidine, pyrazolidine, 1,3-dipolar Cycloaddition, Selectivity, DFT Calculations.

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Development of pH-Sensitive Sodium Alginate Films Reinforced with Cellulose Nanocrystals and Anthocyanin Extract from *Hibiscus sabdariffa* for Intelligent Food Packaging

Ali BENAYAHOUM [a, b], Samia BOUAKKAZ [a], Asma BEHLOUL [a]

[a] Laboratoire de recherche en chimie appliquée (LCA), BP 401. 24000. Guelma.
[b] Centre de Recherche Scientifique et Technique en Analyses Physico-Chimiques CRAPC, BP384, Bou-Ismail, 42004, Tipaza, Algeria.
Corresponding author: ali_benay@yahoo.fr

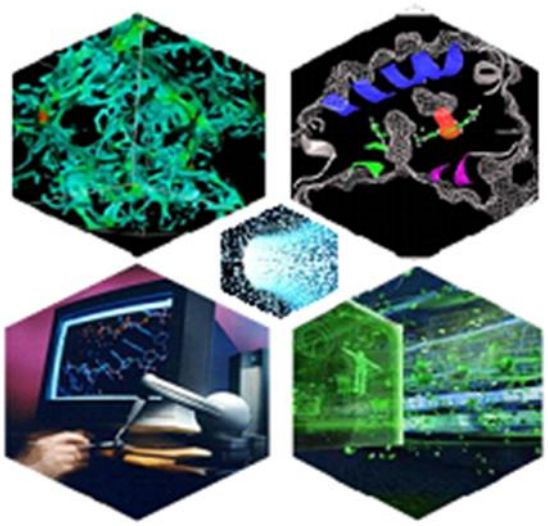
Abstract

This study aimed to develop and characterize pH-sensitive sodium alginate (SA)-based films reinforced with cellulose nanocrystals (CNC) and colored with anthocyanin-rich extract from *Hibiscus sabdariffa* (karkadé). The films were prepared with varying CNC concentrations (100–400 mg) and different extract pH levels (2, 3, and 4.5) to investigate their influence on the films' mechanical, optical, and structural properties. Mechanical testing revealed that CNC addition slightly improved tensile strength, while anthocyanin incorporation led to decreased strength but imparted pH-dependent color changes. The most intense red hues were obtained at pH 2, associated with the flavylium cation form of anthocyanins, whereas higher pH values resulted in lighter violet tones. SEM analysis showed that CNC improved surface compactness and reduced phase separation, while FTIR spectra confirmed hydrogen bonding and electrostatic interactions among CNC, alginate, and anthocyanins. All films displayed complete water solubility and low water activity (Aw < 0.45), ensuring microbiological stability. The integration of CNC and natural pigments provided tunable coloration, enhanced opacity, and reinforced structure, highlighting the synergistic role of nanocellulose and bioactive compounds. These findings demonstrate the potential of *H. sabdariffa*-based anthocyanin films as **biodegradable, intelligent materials** for visual freshness monitoring and active food packaging applications.

Keywords: sodium alginate; cellulose nanocrystals; anthocyanins; *Hibiscus sabdariffa*; pH-sensitive films; intelligent packaging.

Theme 2:

Molecular Modeling and Theoretical Calculations



A MEDT Study on The Mechanism and Reactivity of Diels–Alder Reactions Between Substituted Pyridinones and Ethylenes

Leila Barama[1,2], Lylia NASRI[1,2], AbdelmalekKhorief Nacereddine[2].

[1]National Higher School of Technology and Engineering – Annaba 23000, Algeria
[2]Laboratory of Organic Synthesis and Biocatalysis, Badji Mokhtar University, Annaba 23000, Algeria

l.barama@ensti-annaba.dz

Abstract

A computational study of the regioselectivity and the stereoselectivity of the Diels-Alder cycloaddition reaction between substituted 2-pyridones and ethylenes affording the corresponding lactams [1]. This study was performed within the molecular electron density theory using DFT method at the B3LYP / 6-31G (d) theoretical level [2,3]. Analysis of the global reactivity indices allows us to classify pyridinone **1** and benzyloxyethene **4** as good nucleophiles and nitroethene **3** and pyridinone **2** as strong electrophiles [4]. These reactions characterized by low activation energies, favoring the formation of the ortho-exo cycloadduct according to a relatively polar asynchronous mechanism. Inclusion of the solvent effects decreases the activation energies and increases the exothermic character of all competitive pathways, but the regioselectivity and stereoselectivity of these cycloaddition reactions remain unchanged.

Keywords: Cycloaddition, 2-pyridones, Lactams, MEDT method, DFT calculations.

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A Density Functional Theory Study of The Adsorption and Decomposition of Nitrou Nanoclusters, With A Focus on The Effects of Incorporating Scandium and Titanuim Dopants

Bochra Bencheikh, Meryem Derdare, Nedjoua Cheghib, Abdel-Ghani Boudjahem

Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, BP 401, 24000, Guelma, Algeria

b.bencheikh@gmail.com

Abstract

In this work, density functional theory (DFT) calculations with the B3LYP functional were employed to investigate the adsorption and decomposition of the N_2O molecule over $MSi_{12}C_{12}$ (M = Sc and Ti) nanocages. The results reveal that N_2O is adsorbed onto the $TiSi_{12}C_{12}$ surfaces through its oxygen atom in Orientation 1, facilitating its dissociation into N_2 and surface-bound oxygen species. The adsorption energies indicate that these metal-doped nanocages significantly enhance the catalytic activity for N_2O decomposition. Furthermore, the ease of O_2 desorption from the $TiSi_{12}C_{12}$ surface suggests the regeneration of active sites, making this system highly promising for continuous catalytic applications. The variation in the electronic properties of these nanocages upon N_2O adsorption highlights their potential use as both efficient nanocatalysts and sensors for toxic gas detection. These findings contribute to the development of advanced nanomaterials for environmental remediation and toxic gas mitigation, reinforcing the role of computational chemistry in sustainable and green chemistry applications.

Keywords: DFT calculations, $Si_{12}C_{12}$ nanocage, Toxic gas detection, N_2O molecule.

DFT Insights into the adsorptive and gas-sensing behavior of transition metal(M)-doped (M = Sc, Mo, Rh, Cr and Pd) germanene monolayers

Abdel-Ghani Boudjahem[1, *], Nedjoua Cheghib, Meryem Derdare [1]

[1] Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, Box 401, 24000, Guelma, Algeria.
Corresponding author: boudjahem@yahoo.fr; nedjoua11_c@yahoo.fr.

Abstract.

The stability and electronic properties of pristine germanene (Ger) and transition metal (M)- doped Ge_{55} nanosheets (M = Sc, Mo, Rh, Cr and Pd) were investigated using the Perdew–Burke-Ernzerhof (PBE) functional with Grimme's dispersion correction to account for van der Waals interactions. The sensing performance of these monolayers toward toxic gas molecules, including HCHO, CO, NH_3, H_2S, CH_4 and SO_2 was also examined. Metal doping significantly enhances the surface reactivity of germanene, making it a promising nanomaterial for the adsorption and detection of these gases. The results reveal that the gas molecules preferentially adsorb at the metal sites, with adsorption energies (Eads) ranging from – 6.5 to – 24.7 kcal mol^{-1}, indicating a chemisorption mechanism. Substituting a Ge atom in germanene with a transition metal atom (Sc, Mo, Rh, Cr or Pd) reduces the energy band gap, thereby improving the surface reactivity and sensitivity of the monolayer. Among the doped systems, Pd- and Cr-Ger monolayers exhibit high sensitivity toward CH_4, SO_2, H_2S and HCHO, while Rh- and Mo-Ger show even greater sensitivity to SO_2, H_2S, CH4 and HCHO compared to Cr-Ger. Moreover, the calculated short recovery times indicate that the desorption of gas molecules from the M-Ger surfaces occurs readily, enabling efficient regeneration of the active sites in all monolayers.

Keywords: DFT, germanene, transition metal doping, adsorption, gas sensing performance.

Crystalline structure of tribromoalinine product obtained from X-ray diffraction compared to the calculated molecular conformation (DFT)

Ouarda Brihi [1], Souheyla Chetioui [23]., Merieme Medjani [1], Meroua Hebat.Erahmane. Akkache[1], Sabah Kellou [14]

[1]Laboratoire de Cristallographie, Université Mentouri, Constantine1, Algérie.
[2]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, (CHEMS), Faculté des Sciences Exactes, Département de Chimie, Université des Frères Mentouri, Constantine 1, Algérie.
[3]Faculté de Technologie, Université Mohamed Boudiaf M'sila, Algérie.
[4]Ecole nationale polytechnique de Constantine, Algerie.
E-mail : ouarda.brihi@umc.edu.dz
brihiouarda@gmail.com

The structure of tribromoaniline resolved at room temperature from X-ray diffraction using a single crystal, crystallises in the space group P 21 21 21. The Hirshfeld surface at 293°K was constructed using the dnorm mode, the dark red spots show the strongest interaction in the crystal. The 2D graphs illustrate all the contacts contributing to the SH surrounding the compound. The result of the distribution of the pairs (di, de) and representing the participation of potential contacts in the crystalline structure.

Calculations for optimizing molecular conformation, using density functional theory (DFT) with the help of the Gaussian09 program chain, have led to results very close to the experimental ones with the functional (B3LYP) and the most suitable basis for organic products. The calculations confirm the planarity of the experimentally obtained molecule. Keywords: Diffraction, DFT, Conformation. Hirshfeld surface analysis

Analyse Quantique Des Interactions Métal–Ligand Dans Les Flavonoïdes : Impact Sur l'Activité Antioxydante

Fella Chouarfa [1], Abida Bahloul [2], Nor El Houda Medigue [3]

[1] Département de génie des procèdes, Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université du 8 Mai 1945, Guelma, Algérie
[2] Département de génie des procèdes, Laboratoire de Chimie Computationnelle et des Nanostructures, Université du 8 Mai 1945, Guelma, Algérie.
[3] Laboratoire de Physico-chimie Théorique et de Chimie Computationnelle, Université des Sciences et de la Technologie Houari Boumediene, Bab Ezzouar, Alger, Algérie.
Chouarfa Fella (maissa_anemone@yahoo.fr)

Résumé

Les composés bioactifs naturels suscitent un intérêt croissant en raison de leur potentiel thérapeutique, notamment les flavonoïdes tels que la quercétine et l'apigénine, connus pour leurs propriétés antioxydantes, anti-inflammatoires et anticancéreuses. Leur activité biologique peut être significativement influencée par la complexation métallique, qui modifie leur comportement électronique et structural. Dans cette étude, la modélisation moléculaire et la théorie de la fonctionnelle de la densité (DFT) ont été utilisées pour examiner l'effet de la coordination avec le cuivre sur les propriétés physico-chimiques et antioxydantes de la quercétine et de l'apigénine. Les descripteurs quantiques calculés, tels que l'écart énergétique, l'affinité électronique et l'électrophilicité, montrent que la complexation diminue cet écart, traduisant une réactivité chimique accrue, une meilleure capacité de transfert électronique et une stabilité améliorée. L'analyse des fonctions de Fukui et des orbitales frontières révèle une redistribution de la densité électronique après complexation, suggérant une modification du mécanisme antioxydant. Les résultats indiquent que la coordination favorise le mécanisme de transfert monélectronique (SET) au détriment du transfert d'atome d'hydrogène (HAT), conduisant ainsi à une efficacité antioxydante renforcée. Dans l'ensemble, ces travaux soulignent le rôle essentiel des interactions métal–ligand dans la modulation des propriétés électroniques et biologiques des flavonoïdes et offrent des perspectives prometteuses pour la conception rationnelle de nouveaux agents thérapeutiques.

Mots-clés : Flavonoïdes, Quercétine, Apigénine, Complexes métalliques, DFT.

Study of Half-Metallic Behavior in Fe_2TiZ (Z = As and Sb) Compounds via Density Functional Theory (DFT).

D. Heciri

[1]Department of Physics, Laboratory Studies of Surface and Interfaces of Solid Matter (LESIMS), University Badji Mokhtar of Annaba, Algeria

ABSTRACT

Within the framework of Density Functional Theory (DFT), we conducted an in-depth theoretical study of the Fe_2TiZ (Z = As and Sb) Full-Heusler compounds. We employed the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method, using the Generalized Gradient Approximation (GGA) to treat the exchange-correlation potential. Both compounds crystallize in the ordered cubic $L2_1$ structure (Cu_2MnAl type), belonging to the space group $Fm3m$. Our calculations allowed us to determine the structural, elastic, electronic, and magnetic properties of these materials. The results obtained for the structural and elastic properties are in good agreement with available experimental and theoretical data. The analysis of the band structure reveals that the Fe_2TiAs compound exhibits half-metallic behavior, while Fe_2TiSb is characterized by a state near to half-metal. The calculated total magnetic moment is found to be equal to $1\mu B$ for each compound, and this value is demonstrated to be robust, remaining relatively constant with variations in the lattice parameter approximately in range of

5.60 Å to 5.90 Å.

Keywords: Full-Heusler alloys, Elastic constants, Ab initio calculations, Density functional theory (DFT).

First-principles study of the structural, electronic and thermodynamic properties and hydrogen storage performance of $XRuH_3$ (X = Na, K and Rb) compounds

Djihane AHMEDBEHALIL, Nedjoua CHEGHIB, Abdel-Ghani BOUDJAHEM

[1] Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, Box 401, 24000, Guelma, Algeria.

Corresponding author: djihaneahmedbehalil@gmail.com

Abstract.

Perovskite hydrides have recently emerged as promising candidates for hydrogen-storage applications, prompting increasing research interest in their structural and physicochemical properties. In this work, we systematically investigate the structural stability, electronic and thermodynamic properties of the Ru-based perovskites $ARuH_3$ (A = Na, K and Rb) using DFT calculations. Our results show that all three compounds satisfy the mechanical, dynamical, and thermodynamic stability criteria. The density of states profiles reveal that each of these hydride perovskites exhibits metallic behavior. Mechanical parameters further indicate that $NaRuH_3$ displays ductile behavior, whereas $KRuH_3$ and $RbRuH_3$ exhibit brittle characteristics. The gravimetric hydrogen-storage capacities are predicted to be 2.38 wt% for $NaRuH_3$, 2.11 wt% for $KRuH_3$ and 1.60 wt% for $RbRuH_3$. The corresponding hydrogen desorption temperatures are estimated at 359.9 K, 261.8 K and 175.4 K, respectively. The obtained results suggest that $NaRuH_3$ and $KRuH_3$ are the most promising candidates for practical hydrogen storage applications due to their higher stability and more favorable thermodynamic profiles. Overall, this study contributes new insights into the physical properties of Ru-based hydride perovskites and provides a solid foundation for their potential use in the design and development of efficient hydrogen storage materials.

Key words: Perovskite hydrides, electronic and thermodynamic properties, hydrogen storage.

Comparative Study by The DFT Method Between TB-mBJ and GGA+U On Structural, Electronic, And Optic Properties of Cerium Dioxide: Effect of Oxygen Vacancy

Malika DOGHMANE [1], Sabah CHETTIBI[1], Aida BENMALIK [1]
[1]8 Mai 1945 University, l'aboratoire de physique des matérieux L2PM, Guelma

Corresponding author: malika_doghmane@yahoo.fr

Abstract

This study investigates the structural, electronic, and optical properties of cerium dioxide (CeO_2) doped with samarium (Sm) at different concentrations (0.125, 0.25, 0.50, and 0.75) in the presence of oxygen vacancies. Using advanced density functional theory (DFT) calculations, specifically the WIEN2k package with GGA-WC and TB-mBJ approximations we analyze how Hg incorporation modifies the behavior of CeO_2.

The results reveal that Sm doping significantly alters the band gap and Fermi level of CeO_2, consistent with previous studies on doped oxides. At higher concentrations (0.50–0.75), the band structure is strongly perturbed, leading to band gap narrowing and the emergence of defect-induced states. In contrast, lower concentrations (0.125–0.25) improve the electronic and optical properties, resulting in a more stable gap, fewer defect levels, and enhanced optical absorption in the visible region. The optical properties, including the dielectric function and absorption coefficient, were found to be highly sensitive to Sm concentration. High doping contents introduce pronounced absorption peaks associated with defect-related transitions, whereas lower concentrations exhibit smoother dielectric responses and more efficient light absorption in technologically relevant energy ranges. Such behavior indicates that reducing Hg concentration enhances the functional performance of CeO_2 for applications in optoelectronic devices and energy storage systems. Overall, this work demonstrates the tunability of CeO_2 through samarium doping, confirming that careful control of dopant concentration is critical to optimize its performance. These findings pave the way for further theoretical and experimental investigations into Sm-doped CeO_2 for advanced technological applications.

Keywords: Sm-doped CeO_2, density functional theory (DFT), oxygen vacancies, optical properties, band gap engineering, optoelectronic application

A theoretical study on the phase stability and origin of band gaps in bismuth-based non-centrosymmetric half-Heusler compounds

F. Annane[1,2], S. Lazghed[3]

1Département de Physique, université 20 Août 1955, Skikda, Algeria,

2Laboratoire LPR, Département de Physique, Université d'Annaba, Algeria.

3Physico-Chemistry of Surfaces and Interfaces Research Laboratory (LRPCSI), Department of Physics, University 20 August 1955 of Skikda, Road of El Haddeik LP 26, Skikda 21000, Algeria

Abstract:

This study investigates bismuth-based hH compounds MCoBi (M = Ti, Zr, Hf), using ab- initio density functional theory (DFT) calculations based on the Full Potential Linearized Augmented Plane Wave (FP-LAPW+lo) method. These materials crystallize in a non-centrosymmetric cubic MgAgAs (C1b) type with a space group $F4\,3m$. The obtained formation enthalpies and energy-volume curves for the three different atomic arrangements (α, β, and γ) show that the γ phase is the most energetically favorable phase for the three compounds. The half-Heusler compounds under study are semiconductors, while all constituent elements are metallic. The classical theory of molecular orbitals was used to clarify the semiconducting behavior and elucidate the origin of the band gap in these materials. The key interaction responsible for the formation of the so-called d–d gap in these systems is the hybridization of the higher-valent transition element Co with the lower-valent transition element M. However, the presence of the sp-valent element corresponding to Bi is crucial, as it not only hybridizes with Co and M but also provides a channel to accommodate extra d electrons responsible for the stability and gapping of the electronic spectrum of these Hh systems. The obtained results for the band gap, lattice constant, and other structural and electronic properties show excellent agreement with previously reported theoretical studies and available experimental data.

Key Words: Density functional theory (DFT), Bi-based half-Heusler, Structural properties, Band gap.

Exploring the Anti-Inflammatory and Immunomodulatory Potential of Ajuga Iva: In Silico and In Vitro Insights into COX-2 and PGES-1 Inhibition for Dysmenorrhea Treatment

Farah DJELTI[1]; Sarah LAMARI[2]

[1]biology department, CancerLab, University of Tlemcen, Tlemcen, Algéria.

[2] Biology department, Laboratoiry of molecule sbioactif and applications, university of Tebessa

E-mail : Farah.djelti.net@gmail.com

Abstract

Introduction: Dysmenorrhea, a common inflammatory condition affecting a significant portion of the female population, has long been linked to elevated levels of prostaglandins, specifically PGE2, which contribute to menstrual pain and uterine contractions. This study aims to explore the anti-inflammatory potential of **Ajuga Iva**, a plant with known ethnomedicinal uses, through both **in vitro** and **in silico** methods. The bioactive compounds of Ajuga Iva, including **Apigenin**, **Luteolin**, **Naringenin**, and **Quercetin**, were identified for their interaction with key inflammatory enzymes **COX-2** and **PGES-1**, which are critical in prostaglandin synthesis and dysmenorrhea-associated inflammation.

Methods; Molecular docking simulations were performed to assess the binding affinity of these phytochemicals with COX-2 and PGES-1 (PDB ID: 3DWW and 3LN1). The results showed that all compounds exhibited strong binding affinities, with **Quercetin** displaying the highest binding scores for both enzymes. Additionally, hydrogen bonding and steric interactions with key residues of the target enzymes were observed, confirming the compounds' potential to inhibit the inflammatory pathways involved in dysmenorrhea.

Results: The **in vitro** assays demonstrated significant anti-inflammatory activity, particularly through protein denaturation and heat-induced hemolysis assays, where the methanolic extract of Ajuga Iva showed up to 80.68% inhibition of protein denaturation and 83.41% inhibition of hemolysis at higher concentrations. These findings suggest that Ajuga Iva extracts, through their bioactive compounds, could serve as effective anti-inflammatory agents by targeting the COX-2 and PGES-1 enzymes, offering a promising therapeutic approach to manage dysmenorrhea.

Conclusion: The study highlights the potential of Ajuga Iva, confirmed by both computational and experimental methods, as a natural alternative to conventional anti-inflammatory treatments for dysmenorrhea, with promising implications for broader inflammatory conditions.

Keywords: Ajuga Iva, Inflammation, Molecular Docking, COX-2, PGES-1, Dysmenorrhea, Apigenin, Quercetin.

Numerical And Experimental Investigation of Tin Electrodeposition from Methanesulfonate Medium: Determination of Thermodynamic Parameters

Fatima Kesri [1,2], Abed. Mohamed Affoune [1]

[1]Department of Process Engineering, Laboratory of Industrial Analysis and Material Engineering; University 8 May 1945 Guelma, BP 401, Guelma 24000, Algeria

[2] Department of Chemistry, University Badji Mokhtar-Annaba, Annaba, Algeria

Fatima.kesri@gmail.com

Abstract

In this studY( ), the thermodynamic parameters of tin electrodeposition from a methanosulfonate medium were investigated using cyclic voltammetry. The numerical simulation was conducted based on the combination of the general Butler-Volmer equation and the Nernst low. Three characteristic diagrams were established, corresponding to the dimensionless peak current(Ψp/ Ψp), the half peak width (D $f_{p/2}$) and the peak potential separation (D f_p) as a function revof the dimensionless kinetics parameter (L) and the electron transfers coefficients α. . The numerical data were employed to determine the standard potentials of the tin couple in methanesulfonate medium.

Keywords: Cyclic voltammetry, Numerical simulation, Tin, Electrodeposition, Methanesulfonate medium.

Vibrational and thermodynamic properties of copper halides CuCl, CuBr and their ternary alloys CuCl1-xBrx in B3(ZnS)and B1(NaCl) structures

Souhair Fnides [1], Saliha Karfaf [2]

[1] Physics Laboratory at Guelma, University of Guelma P.O Box 401 Guelma 24000, Algeria

[2] Physics Laboratory at Guelma, University of Guelma P.O Box 401 Guelma 24000, Algeria
Corresponding author: Fnides Souhair (souhir.fnides@gmail.com)

Abstract

The structural, lattice dynamical and thermodynamic properties of copper halides CuCl and CuBr and their ternary alloys3CuCl1-xBrx have been studied using first principles calculations. The density functional perturbation theory (DFPT) and the virtual crystal approximation (VCA) are employed. The variation of the structural parameters, the optical and acoustic phonon frequencies at the high symmetry points, the electronic and static dielectric constants, the Born effective charge are studied as a function of the concentration (x). Using the quasi harmonic approximation the thermodynamic function as specific heat is evaluated $_3$.

Keywords: perovskite, the virtual crystal approximation.

From Structure to Optics: A First-Principles Perspective on Mg_2Si and Mg_2Ge Compounds

Nassima Guechi [1], saliha Karfaf [1]

[1] Faculty of mathematical, informatics and material Sciences University of 08 Mai 1945 Guelma, Algeria

Abstract

In this work, we present a first-principles study of the structural, electronic, and optical properties of Mg_2Si and Mg_2Ge compounds using Density Functional Theory (DFT) within the pseudopotential and plane-wave formalism. The optimized structural parameters are found to be in good agreement with available experimental data, confirming the reliability of the computational approach. The calculated electronic band structures reveal that both Mg_2Si and Mg_2Ge are semiconductors with relatively small indirect band gaps. Furthermore, the complex dielectric functions were computed, and their frequency-dependent behavior was analyzed to provide insights into the optical response of these materials. These results contribute to a deeper understanding of Mg_2Si and Mg_2Ge, which are promising candidates for optoelectronic and thermoelectric applications.

Keywords: Band gap, Dielectric function, Structural optimization, Electronic and optical analysis

Photocatalytic Degradation of Congo Red by (Ce/Al_2O_3) Under Solar Irradiation

Samira GUENDOUZ [1], Meriem CHENOUF [1], Nour Zeghouda HADDAD [1], Rayan BOUCHEBBAT [1]

[1] Department of Process Engineering, Faculty of Technology, University of SKIKDA

Abstract

Water pollution is one of the major environmental challenges of our time, especially due to synthetic dyes that deteriorate water quality and threaten aquatic ecosystems. In response to this issue, heterogeneous photocatalysis emerges as an effective and sustainable method, particularly when combined with solar irradiation. In this context, our study focused on the degradation of Congo Red, a widely used and poorly biodegradable azo dye, using a photocatalyst based on cerium oxide supported on alumina (Ce/Al_2O_3). Several operating parameters were investigated: catalyst mass, H_2O_2 volume, initial pollutant concentration, temperature, and the possibility of reusing the catalyst. The degradation process was monitored using UV/Visible spectrophotometry. The results demonstrated significant efficiency of the Ce/Al_2O_3 system under solar irradiation, with optimal degradation rate of 96% achieved using

0.1 g of catalyst, 1 mL of H_2O_2, and a temperature of 20°C. This study confirms the promising potential of this photocatalyst for treating dye-polluted water.

Keywords: Congo Red, heterogeneous photocatalysis, Ce/Al_2O_3, degradation, solar irradiation.

Optimization of Split Pea- based Media for the Growth of Lactobacillus plantarum through Plackett–Burman and Response Surface Methodological Approaches

KASSAS Zohra

Laboratory of Biochemistry and Applied Microbiology, Department of Biochemistry, Faculty of Science, Badji-Mokhtar University BP12, 23000 Annaba, Algéria

E-mail : z-kassas@hotmail.fr

Lactic acid bacteria play an essential role in biotechnology: food, cosmetic and pharmaceutical industry. There are the most important groups of microorganisms used in the food industry, therefore their growth required rich and complex media based on yeast extract or meat and animal peptones) however these properties are related to their development, which in turn related to culture conditions: composition of culture medium, pH of the medium and agitation. The overal aim of this study is to optimize the growth of Lactobacillus plantarum in pea based medium .

Plackett–Burman design was used to determine the most influential of 9 variables (glucose, lactulose, tween80, K_2HPO_4, sodium acetate, $MgSO_4$, pH, shaking and inoculum size) on the growth of L plantarum BH14. Glucose, lactulose, $MgSO_4$ and shaking had a significant effect on growth of this strain at a 70% confidence level. Glucose, lactulose and $MgSO_4$ showed positive coefficient but shaking had a negative coefficient, Thus shaking was avoided in subsequent experiments. Composite design was used to determine the optimum concentrations of the significant variables. An optimized formulation of nutrition levels was suggested from the software at the following concentrations: 11,59 g/l glucose, 11,59 g/l lactulose and 0,23 g/l $MgSO_4$. Growth of L plantarm was compared to that recorded on the reference medium ‘vegetal MRS’. The results showed that viable counts in the optimized culture medium were significantly higher than those in the vegetal MRS medium.

Exploring the interactions of NSAID drug with COX-2 and TAAH: Insights from Molecular Docking

Nadia LACHI

Laboratory of Computational Chemistry and Nanostructures (LCCN), University 8 Mai 1945 Guelma, Algeria.

Lachi_n@yahoo.fr

Abstract :

Nonsteroidal anti-inflammatory drugs (NSAIDs) represents a heterogeneous class of chemical compounds, its main action is the inhibition of cyclooxygenases (COX-1 and COX- 2) , 2 intracellular enzymes that oxygenate arachidonic acid (AA) to prostaglandin H2 (PGH2). COX-2 also oxygenates the endocannabinoids, 2-arachidonoylglycerol (2-AG) and arachidonoylethanolamide (AEA), to the corresponding PGH2 analogs.

But NSAID-mediated COX inhibition is associated with gastrointestinal toxicity. One potential strategy to counter this toxicity is to also inhibit fatty acid amide hydrolase (FAAH), which hydrolyzes bioactive fatty acid ethanolamides (FAEs) into fatty acids and ethanolamine.

Here, we use molecular docking to study, theoretical elucidation of COX interaction with ARN2508, an NSAID that inhibits both COXs and FAAH with high potency, target selectivity, and decreased gastrointestinal toxicity due to its ability to increase levels of FAEs.

The results and the visualization of the interactions of the ARN2508@enzyme complexes shows a good positioning and a better selectivity within the cavity of COX-2 and FAAH, which is in good agreement with the experimental results.

Key Word: Cyclooxygenases, FAAH, ARN2508, inhibition, molecular docking.

The Selectivity And a Mechanistic MEDT Study of The Competitive Non-Catalysed And Lewis acid Catalyzed [4+2] Cycloaddition Reaction Between 1-Methyl-1-Phenylallene and Methyl Acrylate

Leila Barama[1,2], Lylia NASRI[1,2], AbdelmalekKhorief Nacereddine[2]

[1]National Higher School of Technology and Engineering – Annaba 23000,Algeria

[2]Laboratory of Organic Synthesis and Biocatalysis, Badji Mokhtar University, Annaba 23000, Algeria

l.barama@ensti-annaba.dz

Abstract

The selectivity and the nature of the mechanism of the competitive non-catalysed and Lewis acid $AlCl_3$ catalyzed catalyzed [4+2] cycloaddition reactions of 1-methyl-1-phenylallene (**MPA**) with methylacrylate (**MA**) [1] have been theoretically studied within the Molecular Electron Density Theory using DFT methods at the B3LYP/6-31G(d) theoretical level[2]. DFT reactivity indices indicate that **MPA** is a strong nucleophile and the **LA-MA** complex is a strong electrophile [3]. The coordination of **LA** to **MA** enhance the reaction rate and increase the asynchronicity of the [4+2] CA reaction, and increase the polar character of this cycloaddition reaction, which become demands a relatively low activation energy [4]. Analysis of different energy profiles indicates that this LA-catalyzed CA reactions favour the formation of a mixture of meta regioisomers , in agreement with the experiment.

Keywords: Cycloaddition, Mechanism, Catalyst, Selectivity, DFT calculations, MEDT.

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MEDT Analysis of the Polar, Two-Stage [3+2] Cycloaddition Mechanism of an Azomethine Imine

Lylia NASRI[1,2],Leila Barama[1,3], LoubnaOumamar[4], Abdelmalek Khorief Nacereddine[2]

[1] National Higher School of Technology and Engineering ,23005,Annaba, Algeria

[2] Laboratory of Physical Chemistry and Biology of Materials, Department of Physics and Chemistry, Higher Normal School of Technological Education of Skikda, Azzaba 21300, Skikda, Algeria

[3] Laboratory of Organic Synthesis and Biocatalysis, Badji Mokhtar University, Annaba 23005, Algeria

[4] Applied Biochemistry Laboratory, University of Ferhat Abbas Setif-1 19000, Algeria

l.nasri@ensti-annaba.dz

Abstract

This theoretical study, based on Molecular Electron Density Theory (MEDT) and DFT methods, analyses the mechanism and selectivity of the [3+2] cycloaddition (32CA) reaction between an azomethine imine (AI 12) and p-nitrobenzylidenemalononitrile (NBMN, 13). The analysis of Conceptual DFT reactivity indices reveals that AI 12 is a strong nucleophile and NBMN 13 is a strong electrophile **[1]**, which imparts a high polar character (zw-type) to the reaction and a very low activation energy. In agreement with experimental data, the study confirms that the reaction is completely meta regioselective and exo stereoselective **[2]**. The meta regioselectivity is explained by the favourable interaction between the N1 nucleophilic canter of the AI and the C5 electrophilic canter of NBMN **[3]**, as predicted by the Parr functions. The exo stereoselectivity is justified by more favourable electrostatic interactions and hydrogen bonds in the more compact exo transition state (TS-2-mx) **[4]**. Finally, the topological analysis of the Electron Localization Function (ELF) demonstrates that the mechanism is not concerted, but occurs in a single step via two stages ("two-stage one-step"). The formation of the first N1- C5 bond precedes that of the second C3-C4 bond, characterizing a [2n+2π] process **[5]**.

Keywords: azomethine imines, cycloaddition, DFT calculations, mechanism, molecular electron density theory, selectivity.

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Etude Microstructurale D'alliages Binaires Ni - Fe Electro Deposees Dans Les Milieux : Acide Et Ionique

Rafik Maizi *, Cheghib Nedjoua, Abdel-Ghani Boudjahem et Meryem Derdare

Groupe Computationnelle et Catalyse, Laboratoire de Chimie Appliquée, Université de Guelma, Box 401, Guelma, 24000 Algérie.

*E-mail adresse : rmaizi24@gmail.com

Résumé :

Les alliages de NiFe sont connus depuis un demi-siècle. Ils possèdent des propriétés physique - chimique et en particulier des propriétés magnétiques. Ils ont diverses applications. Notre objectif est l'élaboration par voie électrochimique des alliages Fer-Nickel riches en Nickel électrodéposées sur des substrats de cuivre de haute pureté à partir de milieux acides ou ioniques présentant des propriétés importantes en vue d'applications industrielles.

La première partie est faite au laboratoire LAIGM de l'université de Guelma. Une étude est effectuée en fonction des additifs primaires et secondaires dans un milieu acide, où le bain principal est composé des sels de NiSO4 et FeSO4, l'acide borique (H3BO3).

La deuxième partie a été menée au laboratoire LISM de Reims, France. Les échantillons sont élaborés dans un milieu ionique en utilisant les liquides ioniques dont certains ont été synthétisés au laboratoire LISM et d'autres de vocation commerciale, achetés par ce même laboratoire pour but la préservation d'un environnement (le mois pollué possible) ; les dépôts ont été réalisés en atmosphère libre et à l'intérieur d'une boite à gants pour éviter l'humidité et toute contamination possible.

Les couches minces ont été caractérisées par EDX pour connaitre leurs compositions chimiques, par MEB pour connaitre leurs morphologies et par diffraction des rayons X pour connaitre leurs structures atomiques.

Mots clés : alliages de NiFe, électrodéposition, DRX, EDX et MEB.

Molecular docking prediction of natural lignans as α-amylase inhibitor

Rachida Mansouri[1], Abdeslem Bouzina[2], Zineb Aouf[2], Nadjet Frissou[1]

[1]Environmental Research Center, Alzon, 23000 Annaba, Algeria.

[2]Laboratory of Applied Organic Chemistry, Bioorganic Chemistry Group, Department of Chemistry, Sciences Faculty, Badji-Mokhtar - Annaba University, Box 12, 23000 Annaba, Algeria.

Corresponding author: Rachida Mansouri r.mansouri@cre.dz

Abstract

Diabetes mellitus is a major metabolic disorder of global concern that poses a significant public health challenge worldwide. According to the International Diabetes Federation Diabetes Atlas (11th edition, 2024), approximately 620 million adults aged 20-79 years are living with diabetes. Over the past few decades, extensive research on antidiabetic agents has identified natural products as a crucial source for novel drug discovery. Consequently, the development of new and effective antidiabetic therapies remains a global priority. Among natural compounds, lignans polyphenolic molecules widely distributed in plants have long been recognized for their diverse pharmacological and therapeutic properties. One of the key enzymatic targets in diabetes management is α-amylase, an enzyme responsible for hydrolyzing complex polysaccharides into simpler sugars, thereby elevating blood glucose levels. Inhibition of this enzyme can slow the intestinal absorption of carbohydrates, resulting in a reduction in postprandial blood glucose levels. This mechanism has been established as an effective therapeutic strategy for managing type 2 diabetes mellitus (T2DM). In the present study, the interaction patterns of selected lignans with the α-amylase enzyme were investigated using molecular docking analysis. The docking results revealed that the tested lignans exhibited favorable binding orientations and strong interactions with key catalytic residues of α-amylase, through excellent docking scores of approximately -8 kcal/mol, suggesting a high potential for α-amylase inhibition.

Keywords: Antidiabetic activity, α-amylase, Lignans, Molecular docking.

Approche QSPR Pour La Modelisation Et La Predection Du Seuil De La Detection D´Odeur (ODT) Des Quelque Molecules Odorantes

Mebarka TEKHA[1]

[1]Department of Drilling and Mechanics of Oil Fields, Faculty of Hydrocarbons, Renewable Energies, Earth and Universal Sciences, University of Kasdi Merbah Ouargla, Algeria.

Mebarka.tekha@gmail.com

Abstract

Le Seuil de Détection d'Odeur (ODT) est une propriété chimico-sensorielle capitale en toxicologie environnementale, en qualité de l'air et dans l'industrie des arômes. Connaître l'ODT permet d'évaluer l'impact et la nuisance potentielle des polluants atmosphériques, car la perception humaine peut survenir à des concentrations extrêmement faibles. Il est donc crucial de développer des outils pour prédire cette valeur avec précision, sans recourir systématiquement à des tests sensoriels longs et coûteux.

La prédiction de l'ODT est rendue possible par l'établissement de Relations Quantitatives Structure-Propriété (QSPR). Cette approche établit un lien mathématique entre des propriétés physico-chimiques des molécules, telles que le coefficient de partage octanol/eau (log K_{OW}) et la pression de vapeur (P_V), et des informations sur leur structure, appelées descripteurs moléculaires.

Une étude portant sur 134 molécules odorantes a illustré l'efficacité de cette méthode. En utilisant une régression linéaire, les descripteurs tridimensionnels (3D-MoRSE) ont démontré une capacité prédictive exceptionnelle pour l'ODT, atteignant un coefficient de détermination R^2 de 0.973. Ce résultat, supérieur à celui obtenu avec les descripteurs topologiques R^2 = 0.584 souligne que la configuration spatiale d'une molécule est le facteur déterminant de sa perception olfactive. Ces modèles QSPR représentent donc une technique puissante pour évaluer rapidement le potentiel olfactif et environnemental des composés chimiques.

Les mots clés: descripteurs, odeur, descripteurs moléculaires, QSPR, prédiction

Decoding The Stability–Reactivity Balance in IRON Complexes: A DFT Insight

SARA MERAD[1,*], ABDALLAH ZAITER[1,2], BACHIR ZOUCHOUNE[1,2]

1 Laboratory of Applied Chemistry and Materials Technology, University of Larbi Ben M'hidi – Oum El Bouaghi 04000, Algeria.

2 Research Unit of Environmental Chemistry and Structural Molecular Chemistry, Mentouri University – Constantine 25000, Algeria.

* Corresponding author E-mail address: sara.merad@univ-oeb.dz

Abstract

Several iron-based complexes [$FeBr_2(CNAr_3NC)_2$], [$Fe(CNAr_3NC)_2]_2$, and [$Fe_3(BINC)_6$] were investigated using DFT. Structural optimizations were performed with the GGA BP86 functional, and results were validated with the hybrid B3LYP functional for two spin states (singlet = 0, triplet = 1). The calculations show that the ground state of all studied complexes is the singlet, consistent with experimental data. Furthermore, energy decomposition analysis (EDA) was used to characterize the bonding between the iron and [Ligand] fragments in each complex. The EDA breaks down the interaction energy (E_{Int}) into three components: the Pauli repulsion (E_{Pauli}), electrostatic interaction (E_{Elstat}), and orbital interaction (E_{Orb}).

In all complexes, the interaction is mainly driven by orbital and electrostatic contributions, with [$Fe_3(BINC)_6$] showing the strongest interaction due to its dominant orbital component. In contrast, the mononuclear complex exhibits more ionic character rather than covalent, which aligns with the combined attractive interactions (E_{Elstat} + E_{Orb}). These findings highlight how nuclearity and ligand environment influence the bonding nature and electronic properties of the iron complexes

Additionally, global reactivity indices were calculated to identify the most reactive complex. Based on the data, [$FeBr_2(CNAr_3NC)_2$] is the most electronically stable complex, while [$Fe_3(BINC)_6$] is the most reactive due to its high LUMO energy and high electrophilicity index. Dipole moment values support this trend, with the order: $D_{Fe} > D_{Fe3} > D_{Fe2}$.

Keywords: DFT, spin state, iron-complexes, ground state, EDA.

Hirshfeld Surface Analysis, Molecular Conformation And Docking Investigation Of 4,6-Dichloro-2-Methylpyrimidine

Meriem Medjani[a], Wissame Zemamouche[a], Ouarda Brihi[a], Ali Boudjada[a]

[a]Laboratoire de Cristallographie Département de physique Faculté des sciences exactes, Université Mentouri, Constantine, Algérie.

Abstract

In order to understand the behavior of the methyl radical (CH3), a systematic study is carried out on benzene or cyclic products derived from highly symmetrical molecules substituted by methyl and halogen. In our overall work, we determined on the one hand the crystal structure of 4,6-dichloro-2-methylpyrimidine (DMP2) which is resolved from X-ray diffraction from a single crystal at room temperature.

Using the Crystal Explorer program, we analyzed the Hirshfeld surface, understand the crystal stacking and identified the intermolecular interactions that ensure cohesion in the crystal. In parallel with the experimental study, we undertook theoretical calculations of the conformation of the isolated molecule of DMP2 using the methods of DFT (Density Functionnal Theory) [1]. Optimization calculations of the molecular conformation of DMP2 using the program chain GAUSSIAN09 [2] and the functional MPW1PW91 and the base Lanl2DZ gave a C1 conformation with results very close to the experiment for lengthsand for angles. . The Raman and infrared spectroscopy calculations undertaken from the optimization results using the same functional MPW1PW91 and the Lanl2DZ set of

bases led to frequency values very close to the experimental results. The conformation closest to the experimental results undergoes an additional Docking study to study the therapeutic capacities of DMP2 against anti-oxidant activity and Alzheimer's disease.

Mots-clés : Diffraction, DFT, Surface de Hirshfled, Conformation, Spectroscopie, Docking.

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First-Principles DFT Study of Ag_nMo Nanoclusters for Green Catalysis: Adsorption of SO_2 and H_2S toward Environmental Remediation

Meryem DERDARE, Yasmine mezari, Nedjoua Cheghib, Abdel-Ghani BOUDJAHEM, bochra bencheikh

Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, BP 401, 24000, Guelma, Algeria

meryemderdare30@gmail.com

Abstract

In this study, quantum simulations based on Density Functional Theory (DFT) at the TPSS/SDD level were conducted to explore the structural, electronic, and magnetic properties of silver–molybdenum nanoclusters (Ag_nMo, n = 3, 5, 8). These nanoclusters were investigated as promisinnanomaterials for environmental catalysis through the adsorption of SO_2 and H_2S, two major atmospheric pollutants. The results from first-principles modeling reveal that Ag_3Mo, Ag_5Mo, and Ag_8Mo nanoclusters are energetically stable, with Ag_5Mo exhibiting the widest HOMO–LUMO energy gap (1.515 eV), indicative of high chemical stability. Adsorption analyses show that both SO_2 and H_2S preferentially bind to the molybdenum center, demonstrating its dominant role in molecular activation. The calculated electron affinities suggest a strong ability of these nanomaterials to accept electrons, enhancing their catalytic performance. Moreover, magnetic analyses indicate that the magnetic moment is mainly localized on the Mo atom, reinforcing its contribution to catalytic activity. Overall, this work highlights the potential of Ag_nMo nanoclusters as efficient multifunctional nanomaterials for pollution control, contributing to the advancement of quantum-based design of green catalysts for sustainable environmental applications.

Keywords:

Ag_nMo clusters; SO_2 adsorption; H_2S adsorption; Environmental remediation; DFT calculations.

$GaBe_{11}O_{12}$ Nanoclusters as Potential Nanosensors for Phenytoin Detection: A DFT Study

Nedjoua Cheghib*, Abdel-Ghani Boudjahem, Meryem Derdare

Email: nedjoua11_c@yahoo.fr

Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, Box 401, 24000, Guelma, Algeria.

Abstract.

The structural, electronic, and adsorption properties of $Be_{12}O_{12}$ and $GaBe_{11}O_{12}$ nanocages interacting with phenytoin (Phy) were investigated using DFT at the B3LYP/6-31G(d,p) level. The substitution of Be atom in $Be_{12}O_{12}$ by Ga atom narrows the band gap to 2.61 eV, thereby enhancing its reactivity. Strong adsorption of Phy on $GaB_{11}N_{12}$ clusters (E_{ads} = – 1.12 to – 1.60 eV) indicates an exothermic and spontaneous chemisorption process accompanied by charge transfer (0.20-0.27 e) from Phy to the $GaB_{11}N_{12}$ nanocages. Phy also exhibits strong interaction with $Be_{12}O_{12}$ (E_{ads} = – 1.50 eV) and moderate adsorption on $GaBe_{11}O_{12}$ (E_{ads} = – 0.67 to – 0.83 eV), significantly modifying their electronic structures. QTAIM analysis suggests predominantly noncovalent O···nanocage interactions. In aqueous media, the complexes remain stable with slightly reduced band gaps. Sensitivity and recovery time analyses reveal that $GaBe_{11}O_{12}$ exhibits high sensing efficiency and rapid response, making it a promising nanosensor for the detection of the phenytoin in aqueous environment.

Keywords: DFT, $GaBe_{11}N_{12}$ nanocage, phenytoin, adsorption, sensing performance

Ab Initio Investigation of the Mechanical and Thermodynamic Characteristics of a Double Perovskite

Salima Ouendadji [1,2*], Ali Aissani [3], Lakhdar Benahmedi [3], Fouad El Haj Hassan[4]

[1]Laboratoire des couches minces et interface Université Frères Mentouri Constantine 1 - BP, 325 Route Ain el Bey, 25017 Constantine Algeria
[2]Laboratoire de Physique des Rayonnements, Département de Physique, Faculté des Sciences, Université de Annaba, Algeria.
3Technology and Solids Properties Laboratory, Faculty of Science and Technology, University of Mostaganem (UMAB), Algeria
[4]Basic and Applied Sciences Research Center, Al Maaref University, Airport Avenue, Beirut, Lebanon

*Ouendadji.salima@umc.edu.dz

Abstract

In this study, the mechanical behavior of the cubic niobate–tantalate double perovskite **Li_2NbTaO_6** was explored using first-principles calculations within the density functional theory (DFT) framework based on the FP-LAPW method. The obtained elastic constants (C_{11}, C_{12}, C_{44}) fulfill Born's stability requirements, confirming the mechanical soundness of the compound. The calculated bulk (B), shear (G), and Young's (E) moduli demonstrate that **Li_2NbTaO_6** possesses a compact and mechanically resilient lattice capable of withstanding both volume and shape deformations. The negative Cauchy pressure and Zener anisotropy factor reveal partial covalent bonding and moderate anisotropic behavior. According to the Pugh's ratio ($B/G \approx 1.48$) and Poisson's ratio ($\nu \approx 0.22$), **Li_2NbTaO_6** can be classified as a brittle material. The melting temperature, derived from elastic parameters, confirms good thermal endurance, while the Kleinman parameter ($\zeta \approx 0.30$) provides insights into the internal strain flexibility under stress. Overall, the findings highlight the mechanical robustness and thermal reliability of **Li_2NbTaO_6**, underscoring its potential use in high-temperature and energy- related technologies. This theoretical analysis provides a valuable foundation for future experimental and functional optimization of Nb–Ta-based double perovskites.

Corrélation Entre Les Propriétés Électroniques Et La Stabilité Colorimétrique De La Cyanidine Issue Du Chou Rouge : Approche Expérimentale Et Computationnelle

Gantri Rayene[1], Chouarfa Fella [2], Benhamza Mohamed EL Hocine [3]

[1]Department de génie des procèdes, Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université du 8 Mai 1945, Guelma, Algérie
[2]Department de génie des procèdes, Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université du 8 Mai 1945, Guelma, Algérie
[3]Department de génie des procèdes, Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université du 8 Mai 1945, Guelma, Algérie
Gantri Rayene (rayengant@gmail.com) Chouarfa Fella(Maissa_anemone@yahoo.fr)
Benhamza Mohamed EL Hocine(benhamza.hocine@univ-guelma.dz)

Abstract

Dans cette étude, les anthocyanines ont été extraites du chou rouge (Brassica oleracea var. capitata f. rubra) à l'aide d'une solution hydroalcoolique acidifiée. Le pigment obtenu a été caractérisé par spectroscopie UV–Visible et infrarouge à transformée de Fourier (FTIR) afin d'identifier les groupements fonctionnels caractéristiques des anthocyanines et de confirmer la présence de la cyanidine comme principal composé colorant. Le spectre UV–Visible a révélé une bande d'absorption intense autour de 526 nm, typique du cation flavylium, confirmant la prédominance de la forme rouge à pH acide. Les spectres FTIR ont mis en évidence les vibrations associées aux fonctions hydroxyle et carbonyle de la cyanidine. Afin de mieux comprendre l'influence du pH sur les propriétés électroniques et chromatiques de la cyanidine, une étude théorique a été réalisée à l'aide du logiciel Schrödinger. Les énergies des orbitales frontières (HOMO et LUMO) ont été calculées pour différentes formes de la molécule correspondant à divers pH. Les descripteurs de réactivité ; potentiel d'ionisation (IP), affinité électronique (AI), électronégativité (χ), dureté (η) et mollesse (S), ont été déduits. Les résultats montrent que la cyanidine présente un faible écart énergétique (0,095 eV) à pH 1, indiquant une forte délocalisation électronique et une intensité colorante élevée. Cette configuration correspond à la forme flavylium, stable structurellement dans les milieux acides. Lorsque le pH augmente, le gap énergétique s'élargit, traduisant une réduction de la conjugaison π et une diminution de la stabilité colorimétrique. Cette approche combinée d'analyse spectroscopique et de modélisation moléculaire fournit ainsi une compréhension approfondie du lien entre la structure électronique, la stabilité et la couleur des anthocyanines naturelles du chou rouge selon le pH du milieu.

Keywords: Chou rouge, anthocyanines, cyanidine, pH, DFT.

Computational Insights into the Mechanical Stability, Electronic Structure and Thermodynamic Properties of HfCoBi Half-Heusler.

S. Lazghed[1], F. Annane[2, 3]

[1]Physico-Chemistry of Surfaces and Interfaces Research Laboratory (LRPCSI), Department of Physics, University 20 August 1955 of Skikda, Road of El Haddeik LP 26, Skikda 21000, Algeria.
[2]Département de Physique, université 20 Août 1955, Skikda, Algeria.
[3]Laboratoire LPR, Département de Physique, Université d'Annaba, Algeria.

Abstract:

In this study, the density functional theory (DFT) within the full-potential plane-wave framework, combined with the local density approximation (LDA), including the potential contribution from the spin–orbit interaction of electrons, was employed to investigate the mechanical, electronic, and thermodynamic properties of the HfCoBi half-Heusler compound. This material crystallizes in a non-centrosymmetric cubic MgAgAs ($C1_b$) type with space group $F\bar{4}3m$. The comparison between the calculated equilibrium lattice constants and the theoretical results shows an excellent level of agreement. The calculated elastic constants reveal that the ground-state structure of HfCoBi satisfies the mechanical stability criteria for a cubic system. Our calculated elastic parameters were compared with previously reported studies and found to be in good agreement with the data available in the literature. Our detailed analysis of the electronic properties, based on various indicators such as the band structure and density of states profiles, reveals that the covalent hybridization between the higher-valent transition metal Hf and the lower-valent transition metal Co is the primary interaction responsible for the formation of the d–d energy gap in these systems. However, the inclusion of the sp-valent element plays a crucial role in ensuring the structural stability of these systems. The analysis of the electron charge density reveals that the bonding nature exhibits a combination of covalent and ionic characteristics. Furthermore, the thermodynamic properties were evaluated using the quasi-harmonic Debye model, which was applied to calculate the Debye temperature and heat capacity at temperatures up to 1600 K under a given pressure.

Key Words: Density functional theory (DFT), Half Heusler, Electronic properties, Elastic properties, Thermodynamic properties, Spin-orbit interaction (SOI).

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Theoretical Investigation of Structural, Electronic and Thermodynamic Properties of TiRhSb Ternary Half-Heusler Compound: Insights from DFT Simulation.

S. Lazghed[1], F. Annane[2, 3]

[1]Physico-Chemistry of Surfaces and Interfaces Research Laboratory (LRPCSI), Department of Physics, University 20 August 1955 of Skikda, Road of El Haddeik LP 26, Skikda 21000, Algeria.
[2]Département de Physique, université 20 Août 1955, Skikda, Algeria.
[3]Laboratoire LPR, Département de Physique, Université d'Annaba, Algeria.

Abstract:

This study investigated the half Heusler compound TiRhSb, using the framework of density functional theory DFT within the full potential linearized augmented plane wave (FP-LAPW) method and studied the structural, electronic and thermodynamic properties based on first-principles calculations, with and without spin-orbital coupling (SOC). The structural properties are predicted local density approximation LDA, the calculations reveal that Lattice constants and other structural parameter with experimental and theoretical results LDA approximation. The calculated band structure and the density of states (DOS), indicates a semiconducting nature with indirect narrow band gaps (Γ-X). The bonding nature discussed via the electron charge density plot shows a mixture of covalent and ionic character. Besides, a regular-solution model was employed to examine the thermodynamic stability of the TiRhSb compound. Additionally, the quasiharmonic Debye model was employed to analyse the impact of temperature and pressure on the Debye temperature and heat capacity.

Key Words: Wien2k, Density functional theory (DFT), Half Heusler, Electronic properties, Thermodynamic properties.

E-pharmacophore Modeling, Molecular docking and ADMET screening to Discover Potential Inhibitors of Polymerization of Tubulin

Samir Bouacha[1*], Malika Chenna[2]

[1]Department of technology, Laboratory of water, Renewable Energy and Environment, University of Mouhamed Boudiaf, M'sila, Algeria.
[2]Department of technology, University of Mouhamed Boudiaf, M'sila, Algeria.

Abstract

This research employed standard methods for drug discovery, specifically e-pharmacophore modeling, 3D-QSAR, and molecular docking, to guide and prioritize the creation of new tubulin polymerization inhibitors. These inhibitors were based on derivatives of compounds like colchicine, combretastatin A-4, and others (e.g., sulfonamide, chalcone). The study successfully developed a highly predictive four-point hypotheses of e-pharmacophore model (one hydrogen bond acceptor (A), one hydrogen bond donor (D) and two rings feature (RR)) and a high-quality 3D-QSAR model (validated by strong correlation, r^2=0.837, q^2= 0.766). The docking molecule is utilized to predict the binding mode and find the optimal orientation of the selected active ligands in the site active of a target protein. Finally, ADMET analysis confirmed that the active ligands possessed acceptable drug-like characteristics.

Keywords: E-Pharmacophore, Molecular docking, Insilico ADMET screening, polymerization of tubulin.

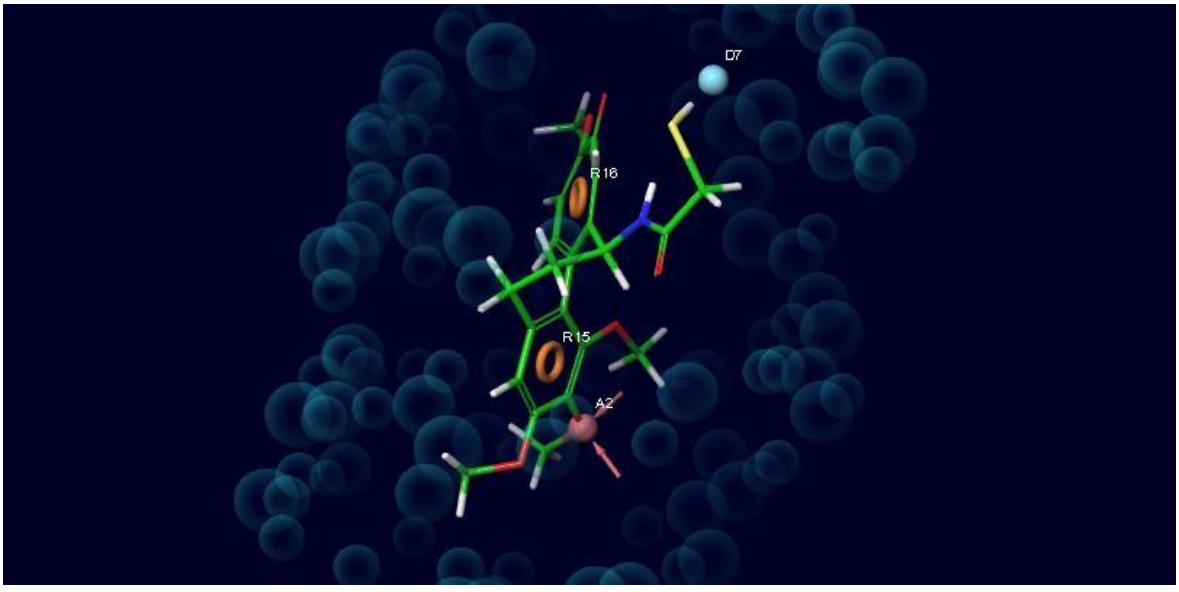

Figure 1. E-pharmacophore model for tubulin mapped onto the native ligand (A2: hydrogen bond acceptor, D7: hydrogen bond donor, R15 and R16: aromatic ring).

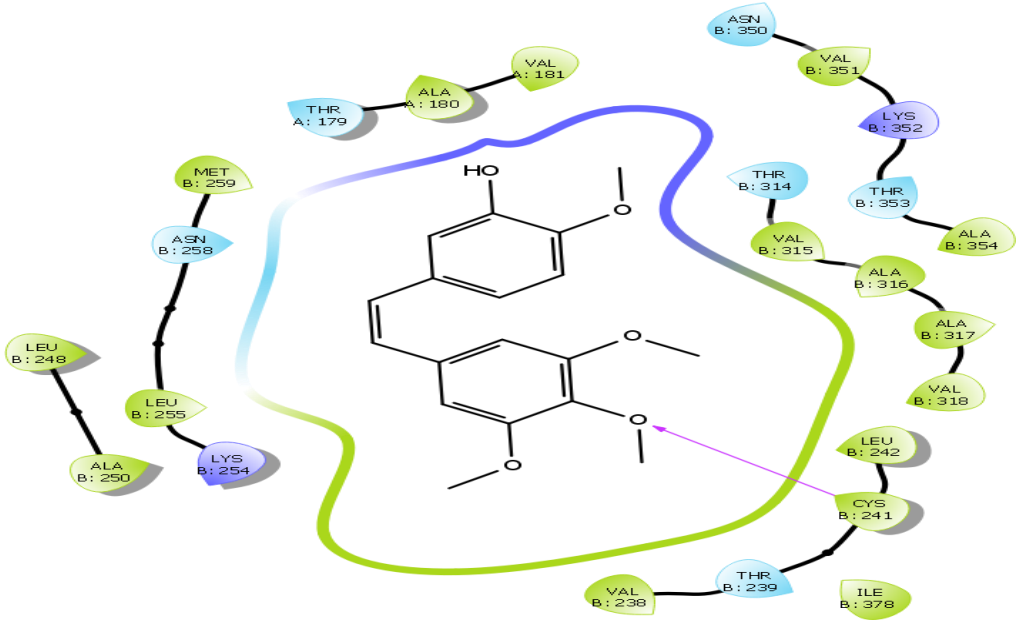

Figure 2: 2D binding interactions of best ligand in the active site of tubulin.

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The Effet of Trihydroxyanthraquinone –Copper Complexation: Structural and Reactivity Insights

Sonia Badi [1], Fatiha Madi[2], Leila Nouar[3]

[1, 2, 3] Laboratory of Computational Chemistry and Nanostructures, University of May 8th, 1945, Guelma, Algeria

Corresponding author: Sonia Badi (badisonia2004@yahoo.fr)

Abstract

To verify the interaction between Trihydroxyanthraquinone and the cupper, several computational analyses were conducted, including molecular electrostatic potential (MEP), frontier molecular orbital (FMO) analysis, reactivity indices, natural bond orbital (NBO) analysis, and a topological study based on the quantum theory of atoms in molecules (QTAIM). The molcular structures were optimized to their energy minima using the density functional theory (DFT) with the hybrid function B3LYP and the 6-311G (d,p) basis set.

Keywords: trihydroxyanthraquinone-Cu, QTAIM, MEP.

Artificial Intelligence (AI) in Drug Design and Discovery

Wafa SOUDANI [1], Nedjoua CHEGHIB [2]

[1]Department of Pharmacy, Laboratory of Organic Chemistry, Badji-Mokhtar Annaba University, Annaba, Algeria.
[2]Department of Materials Science, Laboratory of Applied Chemistry, 8 Mai 45 Guelma University, Guelma, Algeria.
Corresponding author: wafa24soud@gmail.com.

Abstract

Artificial Intelligence (AI) has emerged as a transformative force in drug design and discovery, accelerating and enhancing various stages of pharmaceutical research and development (R&D). This paper explores the integration of advanced AI techniques, including Machine Learning, Deep Learning, Natural Language Processing, Reinforcement Learning, and emerging methods like Quantum Computing, in key areas such as target identification, lead discovery, drug repurposing, lead optimization, and toxicity prediction. Despite these advances, the paper also addresses the methodological limitations, data-related challenges, and potential risks associated with AI applications in pharmaceutical research and development. Overall, we will provide a critical overview of the current landscape, capabilities, and future directions of AI-powered drug discovery.

Keywords: pharmaceutical research, artificial intelligence, drug design, machine learning, deep learning.

Investigation computationnelle du complexe d'inclusion hôte–invité entre la β-cyclodextrine et la 5-fluoro-2-hydroxypyrazine-3-carboxamide

Takoua Belghit[1], Tahar Abbaz[2], Abdelkrim Gouasmia[1]and D. Villemin[3]
1 Laboratory of Organic Materials and Heterochemistry (LOMH), Echahid Cheikh Larbi Tebessi University, Constantine Road, 12002, Tebessa-Algeria.
2 Laboratory of Organic Chemistry and Interdisciplinarity "LCOI", University of Mohamed-Cherif Messaadia, Souk Ahras, 41000, Algeria.
3 Laboratory of Molecular and Thio-Organic Chemistry, UMR CNRS 6507, INC3M, FR 3038, Labex EMC3, ensicaen & University of Caen, Caen 14050, France
E-mail : takoua.belghit@univ-tebessa.dz

Abstract

Le 5-fluoro-2-hydroxypyrazine-3-carboxamide est un composé antiviral reconnu pour sa capacité à inhiber la réplication virale. Dans ce travail, la théorie de la fonctionnelle de la densité (DFT) a été appliquée afin d'étudier le complexe d'inclusion hôte–invité formé entre la β-cyclodextrine (β-CD) et le 5-fluoro-2-hydroxypyrazine-3-carboxamide, aussi bien en phase gazeuse qu'en phase aqueuse.

Les calculs quantiques ont permis d'évaluer et d'interpréter les énergies, les paramètres géométriques. Les possibilités d'interactions intermoléculaires entre le 5-fluoro-2-hydroxypyrazine-3-carboxamide et la β-cyclodextrine ont été analysées à l'aide des méthodes NBO (Natural Bond Orbital) et NCI (Non-Covalent Interactions).
Cette étude théorique fournit des informations complémentaires et utiles sur le phénomène de complexation, difficilement accessible par des méthodes expérimentales.

Keywords : 5-fluoro-2-hydroxypyrazine-3-carboxamide/β-cyclodextrine - DFT – NBO - NCI.

Comparative Study of Molecular Interactions Between COX-2 and Active Principles of Ginkgo biloba and NSAIDs: Approaches by Molecular Docking, DFT, and Molecular Dynamics

Wafaa Taleb Bendiab [1]

[1]medicine, LCPM, University Oran1, Oran, Algeria
tabet.wafaa@gmail.com

Abstract

Cyclooxygenase-2 (COX-2) is an inducible enzyme that plays a key role in inflammatory processes and prostaglandin biosynthesis. Its selective inhibition represents a major therapeutic strategy for controlling inflammation, pain, and related pathologies. However, the adverse effects associated with nonsteroidal anti-inflammatory drugs (NSAIDs) have encouraged the exploration of natural bioactive compounds with safer pharmacological profiles. Ginkgo biloba, a medicinal plant well known for its antioxidant and anti-inflammatory activities, contains several bioactive principles capable of interacting with COX-2. This study aimed to compare the molecular interactions between COX-2 and active constituents of Ginkgo biloba with those of conventional NSAIDs through computational approaches. Molecular docking simulations were carried out to estimate binding affinities and identify key amino acid interactions at the active site. The electronic properties of the ligands were analyzed using Density Functional Theory (DFT) to evaluate their chemical reactivity, and molecular dynamics (MD) simulations were performed to assess the stability of the most stable complexes under physiological conditions. The results demonstrated that the selected natural compounds exhibited favorable binding affinities and stable interactions with crucial residues within the COX-2 active site, comparable to those of reference NSAIDs. Theoretical analyses confirmed their electronic compatibility and conformational stability, suggesting a strong potential for anti-inflammatory activity. These findings highlight the promising role of Ginkgo biloba constituents as natural COX-2 inhibitors and provide a theoretical basis for further in vitro and in vivo validation.

Keywords: COX-2, Ginkgo biloba, NSAIDs, Molecular Docking, DFT, Molecular Dynamics

Electronic and Adsorption Properties of N_2O on $MSi_{12}C_{12}$ (M = Sc, Ti, and V): A Density Functional Theory Analysis

Yasmine MEZARI, Meryem DERDARE, Nedjoua CHEGHIB, Abdel-Ghani BOUDJAHEM

Computational Catalysis Group, Laboratory of Applied Chemistry, University of Guelma, BP 401, 24000, Guelma, Algeria

Email: mezari.yasmine@hotmail.com

Abstract

In this study, density functional theory (DFT) calculations were performed using the B3LYP hybrid functional to examine the electronic and structural behavior of $Si_{12}C_{12}$ nanocages doped with transition metals (Sc, Ti, and V) in both their pristine and N_2O-adsorbed forms. The investigation aimed to evaluate their catalytic potential toward nitrous oxide decomposition by analyzing adsorption characteristics, electronic distributions, and thermodynamic stability. Key parameters such as adsorption energy, HOMO and LUMO energy levels, energy gap (E_g), and other quantum chemical descriptors were computed to elucidate the nature of the interaction and the reactivity of the doped systems. The results highlight the promising role of transition-metal-modified $Si_{12}C_{12}$ clusters as environmentally friendly catalysts, opening pathways for sustainable nanomaterial design and effective mitigation of harmful gaseous pollutants.

Keywords:
DFT calculations; B3LYP functional; $Si_{12}C_{12}$ nanocages; nitrous oxide (N_2O) decomposition

SYNTHESIS, SPECTRAL CHARACTERIZATION, AND THEORETICAL STUDY OF A NEW COUMARIN BASED NICKEL ORGANOMETALLIC COMPLEX

Hayet Belbah[1], Zaineb Ourdjini[2], Karima Belguidoum[1], Fatiha. Madi[3], Leila. Nouar[3], Amira-Guebailia Habiba[1]

[1] Laboratoire de Chimie Appliquée -LCA, Université 8 Mai 1945 Guelma, BP 401, Guelma 24000, Algeria.
[2] Département des sciences de la matière, Université 8 Mai 1945 Guelma, BP 401, Guelma 24000, Algeria
[3] Laboratory of Computational Chemistry and Nanostructure, University 8 May 1945, BP 401, Guelma 24000, Algeria.

Corresponding author: Hayet Belbah (belbahhayet@yahoo.fr)

Abstract

A new nickel organometallic complex was synthesized using Daphnetin, a coumarin isolated from the leaves of Daphne gnidium L. (DGL) plant as ligand. The characterization of the organometallic complex nickel - Daphnetin was carried out by spectroscopic methods (UV-Visible and IR) which showed that a tetradentate square planar organometallic complex between nickel and daphnetin was formed and the metal/ligand interaction took place via the carbonyl group.

To consolidate the results of this experimental study, theoretical calculations were carried out by density functional theory method (DFT). The study of the optimization (energy minima) provided additional proof of the formation of the above mentioned complex and allowed us to determine the most stable structure for the complex. In addition, the determination of the atomic charges, the HOMO and LUMO orbitals as well as the molecular electrostatic potential allowed us to identify the nucleophilic and electrophilic sites within the complex.

Keywords: Daphnetin, Daphne gnidium L., Nickel complex, DFT, UV-visible and FT-IR

In silico Anticancer Activity of Zygophyllum cornutum: Molecular Docking of Selected Apoptotic Target Proteins

Awatif BOUMAZA[1], Fahima TALHI[2], Mouna CHERAIRIA[1], Hayet AYED[1]
1 University of 8 Mai 1945, Guelma, Algeria, 2 University of Abdelhafid Boussouf - Mila, Algeria
awatifboumaza@yahoo.com

Abstract

The incidence of cancer is rising globally. In this study, two phenolic compounds Neocorombosite and Zygophyline from Zygophyllum cornutum are tested in silico to predict their toxicity, pharmacokinetics and their interaction with apoptotic proteins (Caspase-3, Caspase-9, Bax, Bcl-2 and Bcl-xl) by AutodockVina docking software. According to the Km values determined as 0.67 and 0.86 for Neocorombosite and Zygophyline respectively, the kinetics zone determined by Boiled Egg Model, and according to Lipinski rule, the obtained results suggest that these compounds can act as good therapeutic drug for cancer. In silico toxicity results also supports the application of the tested compounds as potential and natural therapeutic agents to treat cancer.

Key words: Apoptosis, cancer, Zygophyllum cornutum, molecular docking.

Analyse DFT-D3 De L'encapsulation Du Dérivé Imidazolyl-Bisphosphonique Dans La B-Cyclodextrine : Perspectives Structurales Et Energétiques

Bouneb Wahiba[1,2], **Bouhadiba Abdelaziz**[1], **Noura Naili**[3,4]

1 Department of Process Engineering, Faculty of Technology, Laboratory of catalysis, bioprocess and environment, University of 20 August 1955, Skikda 21000, Algeria

[2]LRPCSI-Laboratoire de Recherche sur la Physico-Chimie des Surfaces et Interfaces, University of 20 August 1955, Skikda 21000, Algeria

[3]Unité de Recherche de Chimie de L'Environnement Et Moléculaire Structurale (CHEMS), University Constantine (Mentouri), 25000, Constantine, Algeria

[4]Department of Chemistry, Faculty of Science, 20 Août 1955 University, P.O. Box 26, 21000, Skikda, Algeria

E-mail : wahibabouneb@gmail.com

Résumé

Cette étude présente une analyse théorique approfondie de l'encapsulation de l'acide zolédronique (ZA), un dérivé imidazolyl-bisphosphonique, dans la β-cyclodextrine (β-CD) à l'aide de la méthode de la théorie de la fonctionnelle de la densité (DFT-D3). L'objectif principal est d'explorer les aspects structuraux, électroniques et énergétiques du complexe d'inclusion ZA@β-CD afin d'améliorer la biodisponibilité orale du médicament et de réduire ses effets secondaires gastro-intestinaux. Les calculs réalisés montrent que l'encapsulation du ZA dans la β-CD est thermodynamiquement favorable, stabilisée principalement par des interactions non covalentes de type liaisons hydrogène et interactions de van der Waals. Les résultats obtenus ouvrent la voie au développement de nouvelles formulations pharmaceutiques plus efficaces et mieux tolérées.

Mots-clés : Zolédronate ; β-Cyclodextrine ; Complexe d'inclusion ; DFT-D3 ; Interactions non covalentes.

Study of Half-Heusler Alloys ScVX (X = Si, Ge) and Their Application in Spintronics

Gasmi Intissar [1], Khenchoul saleh[2], Hichem Farah[3]

[1] Department of physics, LCAM laboratory of compound and actif Materials, University Larbi Ben Mhedi Oum El bouaghi, Oum El bouaghi ،Algeria.

Gasmi Intissar :(intissarebasset@gmail.com)

Abstract:

Half-Heusler alloys are promising for advanced spintronic applications due to their unique electronic properties. This research focuses on the crystal structure and electronic properties of ScVX alloys where X varies between germanium (Ge) and silicon (Si). Using density functional theory (DFT) calculations with the Wien2k code, we estimated that the bandgap energy for ScVSi is approximately 0.5 eV, while for ScVGe, it is about 0.3 eV. The Fermi level was calculated to be around -4.5 eV for both compounds. These results show that substituting Ge with Si in the ScVX structure can significantly alter the electronic properties, offering prospects for the development of more efficient spintronic devices.
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Keywords : DFT, half métallique matériel, half heusler alloys, Spintronics

Modélisation Moléculaire de la Formation du Complexe : Curcumine / β-Cyclodextrine

Habiba Bouzit[1, 2], Maamar Stiti [1], Sehailia Moussa [2], Nadia Taibi[2], Hamitouche Adh'ya-eddine [2]

[1]Material Sciences, Laboratory of Applied Chemistry, University of Guelma, Guelma, Algeria.
[2] Research Centre in Analytical Chemistry and Physics, University of Guelma, Guelma, Algeria
. Corresponding author: Bouzit Habiba (bouzit.habiba@gmail.com)

Résumé

Dans ce présent travail, nous avons réalisé une investigation théorique au moyen des méthodes de modélisation moléculaire sur l'inclusion du curcumine dans la β-Cyclodextrine (curcumine /β-CD) à la fois en solution et dans le vide. Cette étude fait partie du contexte global de la mise en valeur de la recherche fondamentale dans le domaine de la chimie supramoléculaire et en particulier des nouvelles formulations naturelles dans le secteur pharmaceutique.
La structure et la stabilité du complexe d'inclusion formé ont été déterminées par le traitement des données du processus de complexation, qui a permis de détecter deux types de complexes et à localiser leurs minimums énergétiques.
La caractérisation des deux modèles par les méthodes de modélisation moléculaire a fourni des preuves remarquables de la formation d'un système d'inclusion (curcumine /β-CD) stable.
En outre, l'énergie de complexation, et les investigations orbitales HOMO, LUMO utilisant le niveau de théorie PM3, PM6 confirment cette stabilité. Et en particulier, le modèle B s'est montré plus stable dans le vide et dans l'éthanol.
Enfin, il a été proposé que les principales forces motrices conduisant à la complexation incluent : l'interaction électrostatique et de van-der Waals, l'interaction hydrophobe et la liaison hydrogène.

Mots clés : Curcumine, ß-Cyclodextrine, PM3, PM6, HOMO, LUMO et Modélisation moléculaire

Structural, Electronic and Magnetic Study Comparization between (DMS) BaFMnAs and BaFMnSb

Boumaza Oualid[12].

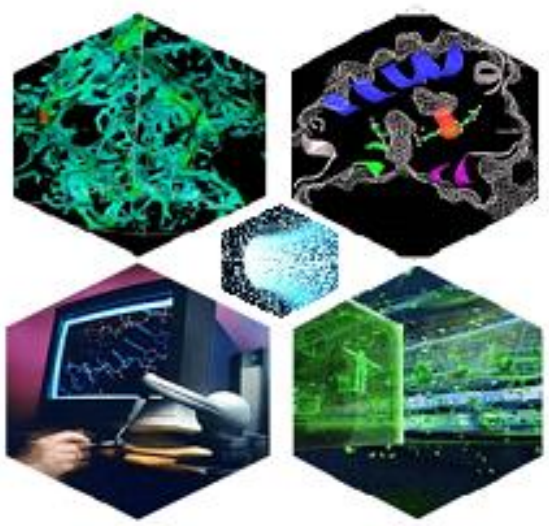
1 Departement of Matter Sciences, Faculty of Sciences and Technology, University Mohamed Cherif Messaadia, Souk-Ahras,
Algeria.
2 Laboratoire de Physique de la Matiere et du Rayonnement, Faculty of Sciences and Technology, University Mohamed Cherif
Messaadia, Souk-Ahras, Algeria.

Abstract:

This study scrutinizes the quaternary compounds BaFMnPn (Pn=As, Sb, Bi), which are poised at the cusp of technological revolution in spintronics due to their unique electronic and magnetic properties. These compounds mirror the structural framework of ZrCuSiAs, and X-ray di raction con rms their crystallization within the tetragonal space group P4/nmm [1]. The novelty of this research lies in the comparative analysis of dilute magnetic semiconductors (DMS) BaFMnAs and BaFMnSb, aiming to dissect the intricacies of their structural, electronic, and magnetic behaviors, and to understand the impact of electronic correlation against the backdrop of changes in exchange energies (Exc) and the substitution of Pn elements. Ab initio simulations uncover that BaFMnPn (Pn=As, Sb) semiconductors exhibit band gaps of 0.6198 eV and 0.0040 eV in the antiferromagnetic phase, and 0.0042 eV and 0.0015 eV in the ferromagnetic phase, respectively. The magnetic properties, denoted by the magnetic spin of Mn atoms, are aptly characterized by the semi-local PBE functional, which closely mirrors experimental data [2]: the ordered magnetic moment for BaFMnAs is computed at 3.561 B/Mn, compared with an experimental value of 3.65(5) B, and 2.537 B/Mn for BaFMnSb, which approaches the experimental value of 3.66(3) B [1]. Emphasizing research in the antiferromagnetic phases, we employ both VASP and Quantum ESPRESSO codes to further delineate the structural, electronic, and magnetic parameters, thereby contributing novel insights to the eld of DMS materials

Theme 3:

Catalysis, Corrosion Chemistry, and Wate Treatment



Etude comparative des propriétés physico-chimiques de l'eau dans la région de Guelma (Nord, Sud, Est, Ouest)

Salma AMRANI[1], Nedjoua CHEGHIB[2], Noor AFAIFIA[3], Imane DERABLA[4]

[1]Faculté FMISM, University 08 mai 45Guelma, Algeria
[2]Faculté FMISM, Laboratory LCA, University 08 mai 45Guelma, Algeria
[3]Faculté FMISM, University 08 mai 45Guelma, Algeria
[4]Faculté FMISM, University 08 mai 45Guelma, Algeria

Abstract

Cette étude s'inscrit dans le cadre de l'analyse des propriétés chimiques de l'eau potable dans la région de Guelma, à travers l'évaluation d'un ensemble d'éléments chimiques essentiels présents dans l'eau, tels que le fer, l'aluminium, les phosphates, le sodium, le potassium, le calcium et le magnésium, ainsi que d'autres ions et minéraux dissous.L'objectif principal est de vérifier la conformité de l'eau aux normes de qualité recommandées par l'Organisation mondiale de la santé (OMS) et les standards nationaux, en s'appuyant sur des références scientifiques fiables telles que Rodier et Technosup pour l'interprétation des résultats analytiques.La méthodologie adoptée repose sur le prélèvement d'échantillons dans différentes zones de la wilaya, suivie d'analyses en laboratoire portant sur les paramètres chimiques ayant un impact direct sur la santé publique et la qualité de l'eau.Les résultats obtenus ont permis d'évaluer l'état actuel de l'eau distribuée, d'identifier les points forts et les insuffisances du système d'approvisionnement et de contrôle, et de proposer des recommandations scientifiques et techniques visant à améliorer la qualité de l'eau et à garantir sa potabilité.Cette étude contribue à soutenir les politiques locales de protection des ressources hydriques, et constitue une référence scientifique utile pour les travaux futurs liés à la qualité de l'eau en Algérie.

Keywords : eau de source, région de Guelma, étude comparative, ADE

Thermo–Iron Co-Activated Inorganic Oxidising Species for Orange G Dye Degradation in Aqueous Media

Nesrine BOUGOUIZI[1], Mahdi CHIHA[2], Fatiha AHMEDCHEKKAT[3], Amina BOUSIREB[4]

[1]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[2]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[3]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[4]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

Corresponding author: Bougouizi Nesrine (bougouizinesrinz@gmail.com)

Abstract

In recent years, considerable research efforts have focused on the removal of persistent organic pollutants from aqueous systems using **advanced oxidation processes (AOPs)**. Among these, the activation of **inorganic oxidising species (IOS)** such as periodate, peroxydisulfate, and peroxymonosulfate has emerged as a promising technique for the generation of reactive oxygen species (ROS). The primary objective of this study is to eliminate of the **azo dye Orange G (OG),** a common pollutant in textile effluents, using a novel **thermo–iron co-activated IOS system.** The results reveal that the amount of energy exchanged plays a crucial role in enhancing the reactivity IOS and the formation of **sulfate** ($SO_4^{\bullet-}$) and **hydroxyl** ($HO^{\bullet}$) radicals. Moreover, activation by heat and transition metal ions, particularly **iron** (Fe^{2+}/Fe^{3+}), significantly improved the oxidative potential of the system. The oxidation kinetics of Orange G were faster in the combined **thermal/OIS** process than in the single activation mode, showing a synergy effect of **68.48%** for the thermal/OIS system and **88.79%** for the **thermal/OIS/iron** process. Furthermore, a **75.41% reduction in chemical oxygen demand COD** was achieved after **260 minutes** of treatment, confirming the efficiency of the thermo–iron co-activated IOS process as a promising AOP for dye degradation in aqueous media.

Keywords: Advanced oxidation process, Inorganic oxidising species, Sulfate radical, Orange G, Wastewater.

Orange G Removal from Aqueous Solution Using Non-Thermal Glidarc Plasma

Nesrine Bougouizi [1], Mahdi Chiha [2], FatihaAhmedchekkat [3], Amina Bousireb [4]

[1]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O.Box 26, 21000, Algeria.
[2]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.
[3]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.
[4]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O.Box 26, 21000, Algeria.

Corresponding author: Bougouizi Nesrine (bougouizinesrinz@gmail.com)

Abstract

Plasma is a complex physicochemical medium whose composition depends strongly on the type of plasmagenic gas employed and the voltage applied between the electrodes. In this study, the oxidation and degradation of the **azo dye Orange G (OG)** were investigated using **non-thermal atmospheric plasma** generated in humid air. Experiments were performed in a **first-generation semi-open batch-type glidarc plasma reactor** designed to evaluate the potential of this advanced oxidation technology for wastewater treatment. The performance of several **gliding arc discharge (glidarc)** configurations was assessed for the removal of OG from aqueous solutions. The reactors operated under **alternating current (AC)** electrical discharges at **50 Hz and 10 kV,** using **two divergent electrodes** positioned in the gas phase above the liquid surface. **UV–Visible spectroscopic analyses** of the treated solutions confirmed effective Orange G degradation, indicating that the formation of highly reactive **hydroxyl ($HO^{\bullet}$)** radicals played a key role in initiating oxidation reactions and producing transient intermediates that were subsequently decomposed. Furthermore, **photocatalytic treatments ($UV/Fe^{2+}/H_2O_2$ and UV/H_2O_2)** achieved complete decolourisation of the dye, demonstrating the synergistic potential of plasma-assisted processes for efficient organic pollutant degradation. These results confirm that **glidarc-based non-thermal plasma** is a promising and energy-efficient approach for the advanced treatment of dye-contaminated wastewater.

Keywords: Non-thermal plasma, Gliding arc, Advanced oxidation process, OG, Water treatment.

Caractérisation des rejets de saumure et l'étude de leur impact environnemental

Houda Hamdaoui [1]

National Higher School of Technology and Engineering, Laboratory, 23005, Annaba, Algeria
Corresponding author: Hamdaoui Houda (h.hamdaoui@ensti-annaba.dz)

Résumé

Le procédé membranaire par osmose inverse est l'une des techniques de dessalement de l'eau de mer les plus prometteuses : Elle porte sur la caractérisation des rejets issus de la station de dessalement Desaladora de Skikda, qui génère une saumure concentrée en sels et métaux lourds, aussi par la présence de produits chimiques utilisés dans le processus de traitement, ce rejet modifie les caractéristiques physico-chimiques de l'eau de mer et peut nuire à l'écosystème, notamment en réduisant le taux d'oxygène dissous et présenter un risque pour l'environnement marin, notamment en cas d'accumulation. Pour limiter ces impacts, il est possible de réduire le volume de saumure produit et d'explorer des méthodes d'élimination plus durables.

Mots-clés : Dessalement, eau de mer, osmose inverse, paramètres physicochimiques, pollution.

Abstract

The reverse osmosis membrane process is one of the most promising seawater desalination techniques: It involves characterising the effluent from the Desaladora de Skikda desalination plant, which generates brine concentrated in salts and heavy metals, as well as chemicals used in the treatment process. This waste alters the physical and chemical characteristics of seawater and can harm the ecosystem, particularly by reducing the level of dissolved oxygen, and pose a risk to the marine environment, especially in the event of accumulation. To limit these impacts, it is possible to reduce the volume of brine produced and explore more sustainable disposal methods.

Keywords: Desalination, seawater, reverse osmosis, physicochemical parameters, pollution

Combined Electrochemical and Surface Characterization (AFM, SEM/EDS) of Urospermum.D Butanolic Extract as an Eco-friendly Corrosion Inhibitor for Carbon Steel in Acid Solution

Sirid Remache [1, 2], Adlene Benyamina [1], Merzoug Benahmed [3], Ayache Boultif [4]

[1] Laboratory of Natural Resources and Management of Sensitive Environments,

University of Oum El Bouaghi, 04000, Algeria.

[2] Centre for Scientific and Technical Research in Physico-Chemical Analysis BP 384, Z.I Bou-Ismail RP 42004, Tipaza, Algeria.

[3] Laboratory of Organic Materials and Heterochemistry, University of Tébessa, 12002, Algeria.

[4] Laboratory of Applied Chemistry and Materials Technology,
University of Oum EL Bouaghi, 04000, Algeria.

Corresponding author: Remache Sirid (sirid40@gmail.com)

Abstract

Green inhibitors are a major advancement in corrosion control systems because they effectively prevent corrosion, lessen the adverse effects of metal deterioration, and support sustainable applications. Green inhibitors can replace conventional, frequently dangerous corrosion inhibitors, resulting in safer industrial operations and improved infrastructure integrity. The main focus of this study is how Urospermum.D butanolic extract (UDBE) inhibits carbon steel (CS) from corroding in a molar HCl solution. Potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) were used to evaluate the extract's anticorrosive properties. To characterize the surface roughness and morphology of (CS) samples with and without (UDBE) in acid media, we used energy dispersive X-ray spectroscopy (EDS), scanning electron microscopy (SEM), and atomic force magnetic microscopy (AFM). By increasing its concentration, UDBE's inhibition efficiency (IE) rose to a maximum of 78.41% at 500 ppm at 298K, but it steadily declined as the temperature rose. The (UDBE) is a mixed-type inhibitor with a predominant anodic effect, according to the (PDP) investigation. The (EIS) study validated the notion that increasing the level of (UDBE) raises the charge transfer resistance (Rct) while decreasing the double layer capacitance (Cdl) as a result of the development of a protective layer on the (CS) surface. This study also emphasizes the efficacy of Urospermum.D butanolic extract (UDBE) from as a green corrosion inhibitor, which is crucial for developing eco-friendly corrosion inhibition methods in acidic environments.

Keywords: Green inhibitor, Urospermum.D, Corrosion, AFM, SEM/EDS.

Dissolution Des Minéraux Carbonatés Mise En Evidence Par L'abondance Des Bicarbonates Dans Les Eaux De Sources (Guelma)

Samia Benrabah [1*], Mouna Cherairia [2], Nedjoua Cheghib [3], Mounira Touati [4]

[1]Department of Geology, Geology Research Laboratory (GRL), Faculty of Earth Sciences, Badji Mokhtar – Annaba University, P.O. Box 12, 23000, Annaba, Algeria.
[*]Email: hydroannaba@hotmail.fr
[2]University of 8 Mai 1945, BP 401-24000, Guelma, Faculty of Natural and Life Sciences, Earth and Universe Sciences, Biology Department, Guelma, Algeria. https://orcid.org/0000-0003-4463-4489
[3]Université 8 Mai 1945, Box 401-24000, Guelma, Computational catalysis group, Applied chemistry Laboratory, Guelma 24000, Algeria
[4]Laboratory of Geodynamics and Natural Resources (LGRN), Department of Geology, Faculty of Earth Sciences, Badji Mokhtar – Annaba University P.O. Box 12, Annaba, 23000, Algeria.

Abstract

L'étude des eaux de sources de la région de Guelma Nord est un cas particulier qui permet de mettre en évidence le processus de dissolution des minéraux carbonatés par la présence et l'abondance des bicarbonates. C'est un exemple concret où la géologie, l'hydrogéologie et la chimie s'associent pour créer un paysage unique et des ressources en eaux caractéristiques. La région de Guelma se caractérise par des formations carbonatées d'âge Eocènes et Crétacé, une structure géologique complexe favorisant la karstification et une présence de sources thermales témoignant de circulations profondes des eaux avant leur apparition en surface. L'ion bicarbonate (HCO_3^-) est le produit direct et majeur de la dissolution du calcaire par l'eau chargée en CO_2. Ce processus de dissolution n'est pas uniforme car l'eau s'infiltre préférentiellement le long de fractures dans la roche, les élargissant progressivement. Cette dissolution crée des paysages karstiques caractérisés par des gouffres et dolines en surface, des réseaux de galeries et grottes souterraines, des rivières souterraines et des résurgences. L'analyse chimique des eaux de sources de la région d'étude issue d'un aquifère carbonaté (un massif calcaire) révèle une forte concentration en ions bicarbonates (HCO_3^-), une forte concentration en ions calcium (Ca^{2+}) et/ou magnésium (Mg^{2+}) (calcite et dolomite), une dureté élevée directement liée à la teneur en calcium et magnésium et un pH généralement neutre à légèrement alcalin (7 à 8,5). Des paramètres secondaires tels que Sulfates (SO_4^{2-}) et Chlorures (Cl^-) sont analysés pour détecter l'influences externes sur ces eaux.

Keywords : sources d'eau, bicarbonates, dissolution, Guelma, thermalisme, Karst.

Biosynthesised Iron Nanoparticles as Efficient Agents for Water Purification

Abderrahim Boutemedjet [1,2], Yehya Bouraghda [3, 4]

[1]Department of Process Engineering, Laboratory of Physics for Matter and Radiation, University of Souk Ahras, Souk Ahras, Algeria
[2]Department of Process Engineering, Laboratory of Environmental Engineering, University of Badji Mokhtar, Annaba, Algeria.
[3]Department of Process Engineering, University of 8 Mai 1945, Guelma, Algeria
[4]Department of Process Engineering, University of Badji Mokhtar, Annaba, Algeria
Corresponding author: Abderrahim Boutemedjet (ab.boutemedjet@univ-soukahras.dz)

Abstract

The increasing discharge of synthetic dyes from textile and industrial effluents poses a serious threat to aquatic ecosystems and human health due to their toxicity, persistence, and resistance to conventional treatment methods. This study investigates the biosynthesis of iron nanoparticles using plant extracts as reducing and stabilising agents, and their subsequent application in dye degradation through the Fenton oxidation process. The green synthesis approach offers an eco-friendly and cost-effective alternative to conventional chemical synthesis, avoiding toxic reagents and harsh reaction conditions. The catalytic performance of the was evaluated in the Fenton reaction for the degradation of synthetic dyes. The results demonstrated rapid dye removal under optimal pH and hydrogen peroxide concentrations, with degradation efficiencies exceeding 90%. The strong catalytic activity is attributed to the large surface area and reactive sites of the biosynthesized. This study highlights the potential of biosynthesized iron nanoparticles as sustainable catalysts for wastewater treatment, offering an environmentally benign and effective approach to the degradation of hazardous dyes through the Fenton process.

Keywords: Green nanotechnology, Iron nanoparticles, Fenton process, Dye degradation, Wastewater treatment.

Impact De Stockage Et Distribution Sur La Qualité Physico-chimique et Bactériologique Des Eaux de Consommation Dans La Région De Guelma

Soumia Abdi [1], Seyf Eddine Merzoug [1, 2], Wissem Mekhania[1], Tayma Chayma Blanchet[1] et Moussa Houhamdi [1]

[1] Université 8 Mai 1945 Guelma, Faculté SNV-STU, département de biologie, Laboratoire Biologie ; Eau et environnement (LBEE), B.P 401, Guelma (Algérie)

[2] Département de biologie, institut de Science de la nature et de la vie, Centre universitaire Abd El Hafid Boussouf Mila

Abstract

Dans le cadre de notre étude, nous avons réalisé des analyses comparatives de la qualité physiques, chimiques et bactériologiques des eaux de source et des eaux de citernes qui sont alimentés par ces source et commercialisés dans la région de Guelma. Afin d'atteindre les objectifs de cette étude ; quatre échantillons ont été prélevés : deux provenant des sources (Ain Souda et Dahwara) et deux autres des citernes alimentées par ces mêmes sources ; afin de déterminer si la qualité de l'eau y était préservée ou non après stockage ; transport et distribution de ces eaux de source par les citernes. Nos résultats ont montré que la majorité des paramètres physico-chimiques analysés répondent aux normes algériennes, donc nos eaux sont de qualité physico-chimique acceptable. Concernant les analyses bactériologiques, les eaux de source de Dahwara présentes une bonne qualité ; Tandis que les eaux de citerne de cette source sont de mauvaise qualité. En ce qui concerne les eaux de citerne de Ain Souda et Dahwara ; les deux présentent une mauvaise qualité dus aux présences des germes totaux ; ainsi que les indicateurs de contamination fécal avec des valeurs dépassent largement les normes de l'OMS pour les eaux de consommations. On a pu aussi montrer la présence de grande variété de germe très pathogènes telle que Pseudomonas aeruginosa ; Serratia odrifera 1 ; Proteus mirabilis, dans les eaux de citerne de Dahwara et Ain Souda. Donc ces eaux sont impropres à la consommation humaine.

Keywords : eau de source, citernes, Ain souda, Dahwara, analyses physico-chimiques, bactériologiques.

Sustainable Synthesis of Schiff Base-Functionalized Nanocellulose from Peanut Shell Waste for Efficient Water Treatment Applications

Khaoula Alia[1], Djamal Atia[2]

[1] Department of Process and Petrochemical Engineering, Laboratory of Biotechnology Biomaterials and Condensed Matter, Faculty of Technology, University of El Oued, 39000, Algeria.
[2] Department of Chemistry, University of El Oued, Algeria.
Corresponding author: ALIA Khaoula (alia.khaoula@gmail.com)

Abstract

This research presents the sustainable synthesis of nanocellulose derived from peanut shell agricultural waste and its functionalization with Schiff base groups for water purification applications. Peanut shells, an abundant yet underutilized biomass, were converted into nanocellulose through sequential chemical delignification and mechanical disintegration, yielding a high-surface-area, biodegradable material rich in reactive hydroxyl groups. To enhance its adsorption efficiency toward organic pollutants, the nanocellulose was chemically modified via Schiff base condensation using aromatic aldehydes, forming imine (C=N) linkages on the polymer backbone. The resulting Schiff base-functionalized nanocellulose exhibited increased surface activity, porosity, and affinity toward cationic dyes. Batch adsorption experiments using Methylene Blue as a model dye demonstrated a removal efficiency of 98%, indicating strong electrostatic and π–π interactions between dye molecules and the functionalized surface. Kinetic and equilibrium studies revealed that the adsorption followed pseudo-second-order kinetics and conformed to the Freundlich isotherm model. Characterization by FTIR and UV–Vis spectroscopy confirmed successful Schiff base formation and dye binding, while SEM imaging illustrated improved surface roughness and structural uniformity. This study highlights the valorization of agro-industrial residues into high-value functional nanomaterials. The integration of nanocellulose and Schiff base chemistry offers a green, low-cost, and regenerable platform for removing organic dyes from wastewater, contributing to the advancement of sustainable water treatment technologies and circular bioeconomy approaches.

Keywords: Schiff base, nanocellulose, peanut shell Waste, water treatment, dyes.

Crosslinked Chitosan–Benzoin Schiff Bases for Efficient Dye Removal in Water Treatment Applications

Khaoula Alia [1], Djamal Atia [2]

[1] Department of Process and Petrochemical Engineering, Laboratory of Biotechnology Biomaterials and Condensed Matter, Faculty of Technology, University of El Oued, 39000, Algeria.
[2] Department of Chemistry, University of El Oued, Algeria.
Corresponding author: ALIA Khaoula (alia.khaoula@gmail.com)

Abstract

This study presents the synthesis and evaluation of novel crosslinked chitosan–Schiff base materials prepared using benzoin as an aromatic crosslinking agent for the removal of synthetic dyes from aqueous solutions. Chitosan, a biodegradable and renewable biopolymer, was chemically modified through Schiff base condensation between its amino groups and the carbonyl functionalities of benzoin, producing a stable and functionalized polymeric network. The incorporation of benzoin enhanced the structural integrity, rigidity, and adsorption capacity of the resulting materials, making them highly effective for water treatment applications. The prepared chitosan–benzoin Schiff base composites were tested for the adsorption of two representative industrial dyes: Methylene Blue and Reactive Blue 19 (RB19). Batch adsorption experiments demonstrated excellent removal efficiencies of 98% for Methylene Blue and 99% for RB19, confirming the strong affinity between the Schiff base sites and the dye molecules. Kinetic analysis revealed that the adsorption process followed a pseudo-second-order model, while equilibrium data were best described by the Freundlich isotherm, suggesting multilayer chemisorption on heterogeneous surfaces. Characterization using FTIR and UV–Vis spectroscopy verified the formation of Schiff base linkages and successful dye adsorption, whereas SEM analysis indicated improved surface morphology and porosity after modification. Furthermore, the materials exhibited remarkable reusability, maintaining over 90% adsorption efficiency after several regeneration cycles. This research highlights the synergistic effect of benzoin crosslinking and Schiff base chemistry in developing eco-friendly, reusable, and high-performance adsorbents for water treatment and environmental remediation.

Keywords: Schiff base, chitosan, benzoin, water treatment, dyes, adsorption.

Fig Leaf Extract as a Green Inhibitor for Mild Steel Corrosion in Acidic Environment: Electrochemical and Gravimetric Investigations

Halima Rahmouni [1], Soraya Nigri [2] and Rabah Oumeddour [2]

[1]Laboratory of Applied Chemistry (LCA), University of 8 may 1945, Guelma, Algeria,

[2]Laboratory of Industrial Analysis and Materials Engineering (LAIGM), university of 8 may 1945, Guelma, Algeria.

Email address:Rahmounihalima45@gmail.com

Abstract:

The aim of this work was to investigate the inhibitive effect of Fig leaf extract (FLE) for the corrosion of mild steel in an acid medium (1 M HCl). The inhibitory efficacy, adsorption, and action mechanism of this prepared inhibitor were assessed using electrochemical and gravimetric measurements. The obtained results have shown that FLE is of a mixed type, follows the Langmuir isotherm, and this inhibitory efficiency reached a maximum of 94%. The formation of an inhibitor film chemically adsorbed was confirmed by the rise in inhibition efficiency as temperature was increased. The SEM technique was applied to examine the morphology of the steel surface.

Keywords: Corrosion inhibition, Electrochemical measurement, Mass loss, by Fig Leaf Extract, Langmuir adsorption isotherm.

Valorization of P plant peel waste as a low-cost biosorbent for organic dye removal

Amine Titah [1], Daoiya Zouied[2], Ibtissam Boussouf [1]

[1] Petrochemical Department, Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria
[2] process engineering department, Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria

Corresponding author: aminetitah@gmail.com

Abstract

This study focused on the biosorption of crystal violet (CV) dye using powdered P peels as a natural biosorbent. FTIR analysis revealed the presence of significant functional groups responsible for dye binding. The results showed that the removal efficiency of a 15 ppm aqueous solution of crystal violet increased with the mass of P peel powder, due to the greater availability of active binding sites. The maximum removal efficiency of 95.78% was achieved with 0.4 g of biosorbent after 130 minutes of contact time. Correspondingly, the crystal violet concentration decreased over time, reaching a minimum value of 0.66 ppm. These findings suggest that reactive species capable of degrading the CV dye were effectively generated during the adsorption process. Overall, pumpkin peel powder exhibited a strong potential as an efficient and eco-friendly biosorbent for the removal and discoloration of crystal violet dye. UV–Vis spectral measurements confirmed the progressive degradation of crystal violet with increasing biosorbent mass (0.1–0.4 g).

Keywords: Biosorption; Crystal violet Dye removal; P peel powder; FTIR analysis.

Towards a Sustainable Synthesis of Fe_3O_4 Nanoparticles with Enhanced Catalytic Properties

Selma Bencedira[1,2], Lamine Djeddi [3], Ikram Boujedri [1]

[1]Environmental Engineering Laboratory (LGE), Department of Process Engineering, Faculty of Technology, University of Badji-Mokhtar-Annaba, PO Box 12, 23000 Annaba, Algeria.
[2]Laboratory of Inorganic Materials Chemistry (LIMC), Department of Chemistry, Faculty of Science, University of Badji-Mokhtar-Annaba, PO Box 12, 23000 Annaba, Algeria.
[3]Advanced Technologies in Mechanical Production Research Laboratory (LRTAPM), Laboratory of, Department of Mechanical Engineering, Faculty of Technology, University of Badji-Mokhtar-Annaba, PO Box 12, 23000 Annaba, Algeria
Corresponding author: Selma Bencedira (selma.bencedira@univ-annaba.dz)

Abstract

The controlled synthesis of Magnetite (Fe_3O_4) is an expanding area of research, particularly in the field of catalysis and environmental remediation. This study investigates the impact of using fresh versus commercial precursors ($FeSO_4$ and $FeCl_3$) for the coprecipitation synthesis of Fe_3O_4. The fresh precursors were recovered from iron components extracted from a discarded fan motor, thereby promoting a circular approach to material reuse. The resulting iron oxides were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS). Catalytic activity was assessed through a Fenton-like process targeting malachite green, a model organic pollutant. SEM images revealed that Fe_3O_4 synthesized from freshly prepared precursors exhibited significantly reduced particle aggregation compared to samples derived from commercial reagents. EDS analysis confirmed the expected Fe and O composition across all samples but highlighted the presence of more impurities in the commercially sourced materials. Fe_3O_4 synthesized from fresh precursors demonstrated superior catalytic efficiency after 60 min of reaction. This work underscores the environmental benefits of reusing waste-derived materials for chemical synthesis. By reducing impurities and enhancing catalytic performance, the use of fresh, recycled precursors supports.

Keywords: Magnetite, Coprecipitation, waste recycling, Fenton-like reaction, Catalysis, Environmental remediation.

Experimental Investigation of Copper Biosorption Using an Endemique brown Alga

Nadjette Bengourna[1], Karima Belguidoum [2], mouna Nacef [3], Imen Kouadri [3], dounia Khalla [3]

[1]Department of Process Engineering, Laboratory of Silicates, Polymers and Nanocomposites (LSPN), University 8 Mai 1945, Guelma, BP 401, Guelma, Algeria.
[2]Department of Process Engineering, Laboratory of Applied Chemistry (L.C.A), University of May 8, 1945, BP 401, 24000 Guelma, Algeria.
[3]Department of Process Engineering, Laboratory of Industrial Analysis and Materials Engineering (L.A.I.G.M), University 8 May 1945 Guelma, BP 401, Guelma 24000, Algeria

Abstract

Polluted water sources with heavy metals are harmful to aquatic life. Humans are doubly impacted by water pollution; directly by the use of contaminated water or indirectly by fish and other sea product consumption. In fact, the harmful accumulative behaviour of such metals in aquatic organisms has been raised by the scientific community over the past decades. This study explores the use of a natural brown alga as an eco-friendly biosorbent for the removal of copper ions (Cu^{2+}) from aqueous solutions. The biosorbent was characterized using FTIR and XRD analyses to identify its main functional groups and structural features. Batch biosorption experiments were conducted to assess the influence of various parameters, including pH, initial copper concentration, contact time, biosorbent dose, and temperature. The results revealed a high copper removal efficiency, with a maximum adsorption capacity of approximately 14.66 $mg \cdot g^{-1}$. These findings demonstrate that brown algae can serve as effective, low-cost, and sustainable biosorbents for the treatment of copper-contaminated wastewater, providing a promising alternative to conventional materials such as activated carbon.

Keywords: Biosoption, Brown alga, Copper, XRD, FTIR.

Orange G Removal from Aqueous Solution Using Non-Thermal Glidarc Plasma

Nesrine Bougouizi [1], Mahdi Chiha [2], FatihaAhmedchekkat [3], Amina Bousireb [4]

[1]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[2]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[3]Chemical Engineering Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

[4]Chemical Department, Laboratory of Anticorrosion-Materials, Environment and structures LAMES-E1061500/TSA & POA-E1061503, Algeria, University of 20 Aout 1955-Skikda, P.O. Box 26, 21000, Algeria.

Corresponding author: Bougouizi Nesrine (bougouizinesrinz@gmail.com)

Abstract

Plasma is a complex physicochemical medium whose composition depends strongly on the type of plasmagenic gas employed and the voltage applied between the electrodes. In this study, the oxidation and degradation of the **azo dye Orange G (OG)** were investigated using **non-thermal atmospheric plasma** generated in humid air. Experiments were performed in a **first-generation semi-open batch-type glidarc plasma reactor** designed to evaluate the potential of this advanced oxidation technology for wastewater treatment. The performance of several **gliding arc discharge (glidarc)** configurations was assessed for the removal of OG from aqueous solutions. The reactors operated under **alternating current (AC)** electrical discharges at **50 Hz and 10 kV,** using **two divergent electrodes** positioned in the gas phase above the liquid surface. **UV–Visible spectroscopic analyses** of the treated solutions confirmed effective Orange G degradation, indicating that the formation of highly reactive **hydroxyl ($HO^{\bullet}$)** radicals played a key role in initiating oxidation reactions and producing transient intermediates that were subsequently decomposed. Furthermore, **photocatalytic treatments ($UV/Fe^{2+}/H_2O_2$ and UV/H_2O_2)** achieved complete decolourisation of the dye, demonstrating the synergistic potential of plasma-assisted processes for efficient organic pollutant degradation. These results confirm that **glidarc-based non-thermal plasma** is a promising and energy-efficient approach for the advanced treatment of dye-contaminated wastewater.

Keywords: Non-thermal plasma, Gliding arc, Advanced oxidation process, OG, Water treatment.

In Situ Growing of Copper Hydroxide on Copper Wire for Acetaminophen Detection

Mouni Boukour*[1], Mouna Nacef [1], Mohamed Lyamine Chelaghmia[1], Abed Mohamed Affoune [1]

[1] Industrial Analysis and Materials Engineering Laboratory, Department of Process Engineering, Faculty of Science and Technology, University May 8, 1945 Guelma, BP 401, 24000 Guelma, Algeria.

*Corresponding author E-mail boukour.mouni2022@gmail.com

Abstract

Emerging pollutants encompass several kinds of anthropogenic chemicals such as cosmetics, pharmaceuticals, pesticides, and household care products. Among them pharmaceuticals are gaining an increasing interest due to their occurrence in the environment. Since the last two decades a great deal of effort is put into the detection and analysis of trace pollutants. Contamination of acetaminophen, a primary analgesic and antipyretic, was wide spread in the water system that affects the ecosystem. No less than 4 % of the administered dose is excreted in the urine. Here's how acetaminophen, as well as other pharmaceuticals are found in soil and waters affecting aquatic organisms, environmental, and human health. In this study, an electrochemical sensor based on copper wire was used for acetaminophen detection. Copper hydroxide was grown in situ using ten cycles in 0.1 M NaOH at the scan rate of 50 mVs^{-1} and used as prepared for electrochemical determination of acetaminophen in alkaline media. acetaminophen detection was revealed by an increasing anodic peak at 0.49 V vs. Ag/AgCl related to an increasing in acetaminophen concentration. The experimental findings proved that the very low-cost and easy to prepare electrode can is capable of sensing acetaminophen.

Keywords. Paracetamol; Sensor; Copper; Cyclic Voltammetry; Emerging Pollutants.

Enhanced Photocatalytic Degradation of Azo Dye using TiO_2 coated Magnesium via Electrophoretic Deposition

Amina Bousireb [1], Fatiha Ahmed Chekkat [2], Mahdi Chiha [3], Nesrin Bougouizi[4]

[1]Laboratory of Anticorrosion-Materials, Environment and structures (LAMES_1061500), Chemical Department, Faculty of Science, University of 20 Aout 1955-Skikda, P.O. Box 26,21000 Skikda, Algeria,

[2]Laboratory of Anticorrosion-Materials, Environment and structures (LAMES_1061500), Chemical Engineering Departement, Faculty of technology, University of 20 Aout 1955-Skikda, P.O. Box 26,21000 Skikda, Algeria

[3]Laboratory of Anticorrosion-Materials, Environment and structures (LAMES_1061500), Chemical Engineering Departement, Faculty of technology, University of 20 Aout 1955-Skikda, P.O. Box 26,21000 Skikda, Algeria,

[4]Laboratory of Anticorrosion-Materials, Environment and structures (LAMES_1061500), Chemical Department, Faculty of Science, University of 20 Aout 1955-Skikda, P.O. Box 26,21000 Skikda, Algeria,

Email.: a.bousireb@univ-skikda.dz

Abstract

In this work, TiO_2 nanoparticles were successfully deposited on magnesium (Mg) substrates by electrophoretic deposition (EPD) and evaluated for their photocatalytic efficiency under UV irradiation. The study aimed to investigate the influence of the metallic Mg substrate on the photocatalytic activity of TiO_2 in comparison with TiO_2 nanoparticles alone. Acid Yellow 99, a representative azo dye, was selected as a model pollutant to assess degradation performance. Structural characterization confirmed the presence of TiO_2 coatings with uniform coverage on the Mg surface, while the XRD pattern revealed the dominance of Mg peaks due to substrate masking effects. The photocatalytic tests demonstrated that the Mg/TiO_2 composite exhibited a significantly enhanced degradation rate compared to TiO_2 alone, which is attributed to the interfacial electron transfer between TiO_2 and the Mg substrate. The metallic Mg facilitated charge separation and suppressed electron–hole recombination, thereby increasing the generation of reactive oxidative species responsible for dye breakdown. These findings highlight the synergistic role of Mg as both a structural support and an electron donor, suggesting that Mg–TiO_2 systems could serve as efficient and low-cost photocatalytic materials for wastewater treatment applications.

Keywords: photocatalytic degradation; Mg/TiO2, electrophoretic deposition, acid yellow 99, uv photocatalysis.

Eco-Friendly Synthesis of ZnO and Ag/ZnO Nanocomposites Using MV Leaf Extract: A Green Approach for Crystal Violet Degradation

Daoiya Zouied [1], Malika Khelfaoui [1], Karima Bekouche[2]

[1] process engineering department, Laboratory of Chemical Engineering and Environment of Skikda (LGCES), University-20 Aout-1955-Skikda, Algeria
[2] process engineering department, University-20 Aout-1955-Skikda, Algeria
Corresponding author: d.zouied@univ-skikda.dz

Abstract

The search for a cost-effective and environmentally friendly method for wastewater treatment is a global challenge. Therefore, in this work, we studied the removal of pollutants from wastewater using zinc oxide, silver, and zinc-doped silver (20/80) nanoparticles synthesized from leaf extracts of the algae plant. IR, UV-Vis, and DRX characteristics demonstrate the formation of these nanoparticles. Finally, we used the synthesized products to degrade an aqueous solution of crystal violet (15 ppm). The results obtained show that the photodegradation efficiency of the dye in the presence of zinc oxide, silver oxide, and zinc-doped silver increases over time, reaching 77.27% at 0.3 g of zinc oxide; 98.14% at 0.2 g of silver oxide; and 98.26% at 0.3 g of silver/zinc (20/80). The aim of using this mixture is to reduce the use of silver, due to its high cost, and increase the degradation efficiency. Finally, we tested the nanoparticles in wastewater treatment.

Keywords: MV leaves extract, AgO. ZnO, Ag/ZnO, Crystal Violet.

Valorization Of Algerian Natural Resources: Phytochemical Analysis And Antibacterial Potential Of A Cultivated Plant

Nedjla Derbal [1]*, Zineb Bouamrane [1], Soumia Bouzidi [1], Hakima Belattar [1] & Abdelfettah Gherib [2]

[1] Laboratory of Natural Sciences and Materials, University Centre Abdelhafid BOUUSSOUF-MILA, Algeria

[2] Centre de recherche en Biotechnologies- CRBT- CONSTANTINE

n.derbal@centre-univ-mila.dz

Abstract

For millennia, medicinal plants have been valued for their curative properties and remain a cornerstone of traditional medical systems worldwide. Owing to its privileged geographical position, Algeria is endowed with diverse and abundant flora. This exceptional biodiversity represents a crucial focus for ethnobotanical and traditional pharmacopoeia research, while also holding significant promise for the valorization of the country's natural resources. Within this context, this study was designed to conduct a phytochemical analysis and evaluate the antibacterial activity of lemon balm (Melissa officinalis L.). This medicinal plant, recognized for its significant bioactive properties, was cultivated in the Zéghaia region (wilaya of Mila). The antibacterial activity of hydro-ethanolic extracts from the aerial parts of the plant was assessed using the agar disc diffusion method, which measures the zone of inhibition around the discs. Qualitative phytochemical screening revealed that the plant is rich in secondary metabolites, including polyphenols, flavonoids, tannins, and alkaloids. Antibacterial assays demonstrated variable and moderate susceptibility of the tested bacterial strains to the different extracts, with inhibition zones ranging from 6.20 to 12.30 mm. At a concentration of 100 mg/mL, the most significant effects were observed against the Gram-negative bacteria Pseudomonas aeruginosa (12.30 ± 0.173 mm) and Escherichia coli (11.15 ± 0.082 mm). In contrast, the Gram-positive strain Micrococcus luteus was largely non-susceptible to the extracts, exhibiting only a minor zone of inhibition (6.20 ± 0.34 mm). These findings indicate that Melissa officinalis L. could serve as a promising source for the extraction and purification of phytochemicals with beneficial health effects, suggesting its potential in preventing various pathological processes.

Keywords: Melissa officinalis L., phytochemical screening, antibacterial activity, hydro-ethanolic extract, lemon balm.

Evaluation of the Compliance of Treated Wastewater from the Baraki WWTP with Agricultural Irrigation Standards

Wafa Djemil [1], Tahani Derradji [1], Hamza Ouaret [1]

1 University 8 May 1945 Guelma, Algeria

Corresponding author: Djemil Wafa (djemil.wafa@univ-guelma.dz)

Abstract

The discharge of wastewater into the natural environment leads to significant pollution and water resource wastage, affecting the quality of surface and groundwater, biodiversity, and human health. To mitigate these adverse effects, it is essential to treat wastewater and promote its reuse, thereby contributing to the preservation of public health, the environment, and water resources. This study focuses on the Baraki Wastewater Treatment Plant (WWTP), which processes domestic and industrial effluents from seven municipalities located in the southern part of the capital. The treated wastewater is then discharged into the Bay of Algiers via the El Harrach River. The main objective of this research is to assess the impact of reusing treated wastewater from the Baraki WWTP for agricultural purposes and to identify its potential environmental risks. A comparative analysis of physico-chemical parameters and heavy metal concentrations was conducted, comparing them to Algerian standards, those of the WHO, and FAO recommendations for irrigation. The results show that, despite the general compliance of most parameters with the recommended standards, some values—particularly ammonium, phosphates, total phosphorus, cadmium, and total chromium (for long-term irrigation)—exceed the permissible limits. In conclusion, this study reveals that the treated wastewater from the Baraki WWTP is not suitable for irrigation due to its potential negative environmental impacts.

Keywords: Treated wastewater, impact, irrigation, pollution, WWTP, reuse.

How Zinc adsorption is influenced by co-occurrence of other heavy metals?

Dounya Khalla*[1], Mouni Boukour[1], Mouna Nacef [1], Mohamed Lyamine Chelaghmia[1], Abed Mohamed Affoune [1]

[1]Laboratoire d'Analyses Industrielles et Génie des Matériaux, Université 8 Mai 1945 Guelma, BP 401, Guelma 24000, Algeria.

*Corresponding author E-mail: dounya.khalla.2021@gmail.com

Abstract

Despite significant technological progress and stricter regulatory measures, the pollution resulting from various industrial activities persists and is exacerbating the decline of water resources. Industrial effluents laden with heavy metals like nickel, copper, lead, cadmium, and zinc pose severe risks to human health. Over the last thirty years, considerable research has been dedicated to understanding the adsorption mechanisms of heavy metals from aqueous solutions. Yet, most investigations have focused on the adsorption of individual metal ions. In reality, wastewater typically comprises a mixture of multiple metal ions. Considering the composition of species present in the related effluents, several scenarios can be envisaged: i) a synergistic effect, where the adsorption of species is enhanced, ii) an inhibitory effect, where the adsorption of certain heavy metal ions is impeded, or iii) a general attenuation, resulting in a reduction of adsorption for all species involved. This study investigated the adsorption of zinc ions under both single-metal and multi-metal conditions, with nickel and cadmium ions concurrently present alongside zinc ions. Activated carbon derived from chestnut shells served as the adsorbent. The findings revealed that the presence of nickel and cadmium in the synthetic solution markedly reduced the adsorption of zinc ions when compared to a scenario involving only zinc ions. A plausible competition for the active sites onto the activated carbon between the heavy metals depending on the heavy metals ions radius, their hydrated diameter and electronegativity might be the cause for the hindrance of zinc ions adsorption.

Keywords: Adsorption; Heavy Metals; Activated Carbon; Water Treatment; Competition.

Photocatalytic Behavior of TiO_2/rGO Nanohybrids in Crystal Violet Degradation

Noureddine Khellaf [1, 2], Khaoula Haouli [2]

[1] Materials Physico-chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid - El Tarf University, P.B. 73, El Tarf 36000, Algeria.
[2] Laboratory of Energetics and Solid-State Electrochemistry (LEES), Department of Process Engineering, FERHAT Abbas University Setif-1, Setif 19000, Algeria
Corresponding author: Khellaf Noureddine (n.khellaf@univ-eltarf.dz)

Abstract

TiO_2/rGO nanohybrids were prepared using the green sol–gel method, where a plant extract served as both the reducing and stabilizing agent. The research generated was directed to both the structural characterization and photocatalytic activity of the prepared nanocomposites for the degradation of the organic dye Crystal Violet (CV) under UV light irradiation. The TiO_2/rGO nanohybrids were subjected to several analysis techniques for determining morphology, crystallinity, and interfacial interaction between the TiO_2 nanoparticles and rGO sheets. The photocatalytic activity of the nanohybrids was significantly greater than pristine TiO_2, with near-complete degradation of CV within a very short irradiation time. This improvement is due to the better electron transfer from rGO, which has the effect of inhibiting the recombination of photogenerated charge carriers and enhancing the overall quantum efficiency. The outcomes advocate for the incorporation of rGO within TiO_2 matrices using a clean synthesis route towards improved photocatalysts, a green and effective route to the elimination of organic pollutants in wastewater.

Keywords: TiO_2/rGO nanohybrids, photocatalysis, Crystal Violet, green synthesis, sol–gel method, UV degradation.

Experimental Evaluation of a Zwitterionic Iminium–Enolate Schiff Base as an Acid Corrosion Inhibitor for Carbon Steel

Leila Lamia Allouche [a, b] , SihemBoufas [a, b], Amel Djedouani [e,f]

(a) Laboratoire de Génie mécanique et Matériaux, Faculté de Technologie, Université de Skikda, 21000, Algeria

(b) Département de Technologie, Université de Skikda, 21000 Skikda, Algeria

(e) Ecole Normale Supérieure de Constantine, Ville Universitaire Ali Mendjeli, Constantine, 25000 Constantine, Algeria 1M

(f) Laboratoire des Produits Naturels d'Origine Végétale et de Synthèse Organique, Faculté des Sciences Exactes, Université des Frères Mentouri-Constantine 25000, Algeria

Abstract:
A new zwitterionic iminium–enolate Schiff base derivative, **3-{(E)-1-[(3-chlorophenyl)iminiumyl]ethyl}-6-methyl-2-oxo-2H-pyran-4-olate**, was synthesized and characterized using **IR** and **^{1}H NMR spectroscopy.** The corrosion inhibition performance of this compound for **carbon steel** in **1 M H_2SO_4** was investigated by **Tafel polarization** and **adsorption studies.** The inhibitor exhibited a maximum efficiency of **82% at 600 ppm**, showing strong protective action against acid corrosion. Electrochemical measurements revealed that the compound acts as a **mixed-type inhibitor**, affecting both anodic and cathodic reactions. The adsorption of inhibitor molecules on the steel surface followed the **Langmuir adsorption isotherm**, with a standard free energy of adsorption (ΔG_{ads}) of **–28 kJ·mol^{-1},** confirming a spontaneous and stable adsorption process. Furthermore, **SEM (Scanning Electron Microscopy) analysis** confirmed the formation of a compact and uniform protective film on the steel surface in the presence of the inhibitor, supporting the electrochemical findings. These results demonstrate that the zwitterionic iminium–enolate Schiff base forms a stable and efficient protective layer, significantly reducing corrosion rates. This study highlights its potential as a **promising organic corrosion inhibitor** for carbon steel in acidic environments.

Keywords: zwitterionic Schiff base; iminium–enolate; corrosion inhibition; carbon steel; sulfuric acid; Langmuir adsorption; Tafel polarization; SEM analysis

Influence of Substituent Nature and Position on the Electrochemical Behavior of 1,2-bis(2-bromobenzylidene) hydrazine (BBBH) as an Organic Corrosion Inhibitor

Laila Lamia Allouche [a, b] , Sihem Boufas [a, b], Amel Djedouani [e,f]

(a) Laboratoire de Génie mécanique et Matériaux, Faculté de Technologie, Université de Skikda, 21000, Algeria
(b) Département de Technologie, Université de Skikda, 21000 Skikda, Algeria
(e) Ecole Normale Supérieure de Constantine, Ville Universitaire Ali Mendjeli, Constantine, 25000 Constantine, Algeria 1M
(f) Laboratoire des Produits Naturels d'Origine Végétale et de Synthèse Organique, Faculté des Sciences Exactes, Université des Frères Mentouri-Constantine 25000, Algeria

Abstract

The efficiency of organic corrosion inhibitors is strongly dependent on their molecular structure, particularly on the nature, position, and presence of substituents on the aromatic ring. These structural factors directly influence the electronic properties, reactivity, and adsorption ability of the molecules on metallic surfaces. In this context, the present study focuses on the compound 1,2-bis(2-bromobenzylidene)hydrazine (BBBH) and its modified derivatives, aiming to evaluate the impact of both the bromine substituent position and the introduction of a hydroxyl group (–OH) on their inhibitory performance against the corrosion of aluminum in an acidic medium (1 M H_2SO_4). Two main aspects were investigated: first, the effect of bromine position (comparison between ortho- and para-substituted BBBH isomers), and second, the influence of hydroxyl group introduction, a highly polar substituent containing an oxygen atom that can increase the electronic density of the compound. These structural modifications are expected to enhance the interaction between the inhibitor molecules and the metal surface, promoting better adsorption and the formation of a stable protective film. Electrochemical investigations were performed using Tafel polarization curves and Electrochemical Impedance Spectroscopy (EIS). Tafel plots were used to determine corrosion kinetic parameters such as corrosion potential and corrosion current, while EIS provided information on charge transfer resistance and the quality of the protective film formed on the surface. The obtained results highlight the correlation between molecular structure and electrochemical behavior of BBBH derivatives, demonstrating that both the position and the nature of substituents (bromine and hydroxyl) play a crucial role in improving inhibitory efficiency. This study contributes to the rational design of new, more efficient organic corrosion inhibitors.

Keywords : corrosion, aluminum, benzylidene derivate, substituents, position, hydroxyl, bromine, Tafel, EIS, organic inhibitors,

Conception D'un Capteur Non Enzymatique Sensible Et Sélectif Pour La Surveillance Du Glucose

Lilia Bourouba[1,2], Messaoud Benounis [1], Emna Zouaoui[3]

[1] Laboratoire des Capteurs, Instrumentation et Procédés (LCIP), Département de Génie des Procédés, Faculté de Technologie, Université Abbes Laghrour, Khenchela
[2] Laboratoire de Recherche en Physico-Chimie des Surfaces et Interfaces (LRPCSI), Département de Génie des Procédés, Faculté de Technologie, Université du 20 Août 1955, Skikda
[3] Laboratoire de Catalyse, Bioprocédés et Environnement, Faculté de Technologie (LCBE), Université du 20 Août 1955, Skikda

l.bourouba@univ-skikda.dz

Abstract

La glycémie est le maître du diabète Les méthodes de détection conventionnelles utilisant des capteurs enzymatiques à base de glucose oxydase (GOx) souffrent de limitations importantes telles que la sensibilité à la température et au pH et la dégradation.
Pour pallier ces inconvénients, une autre solution a été développée : un capteur électrochimique non enzymatique. Ce capteur est constitué d'une pâte de carbone modifiée par des nanoparticules d'oxyde de cuivre (CuO) enrobées de chitosane. Les nanoparticules de CuO confèrent des propriétés électrocatalytiques, tandis que le chitosane améliore la biocompatibilité et la conductivité du capteur, améliorant ainsi sa performance.
Les performances de ce nouveau capteur ont été évaluées par voltamétrie à onde carrée (SWV) et spectroscopie d'impédance électrochimique (EIS). Les résultats indiquent : Une bonne linéarité pour la détection du glucose, dans la plage de 0,05 à 10 mM. Une limite de détection basse, 2,3 µM, sensibilité élevée de 178,5 $\mu A \cdot mM^{-1} \cdot cm^{-2}$. bonne stabilité, reproductibilité et sélectivité vis-à-vis des interférents courants tels que l'acide ascorbique, la dopamine et l'acide urique.
En définitive, ce capteur non enzymatique est une alternative pour les appareils de diagnostic et de surveillance du glucose.

Mots clés : capteur, détection, CuO, sensibilité, spectroscopie d'impédance.

Title of the Paper: Application of Response Surface Methodology for Optimizing Cadmium Adsorption on Chitosan–Activated Carbon/ZnO Composite Beads

Mohammed Rabeh Makhlouf [1], Malek Bendjaballah [2], Imane Ghouafria[3]

[1] Laboratoire d'Analyses Industrielles et Génie Des Matériaux, Université 8 Mai 1945 Guelma 24000, BP 401, Guelma, Algeria

Corresponding author: makhlouf.mohammedrabeh@gmail.com

Abstract

In this study, a novel bio-adsorbent was synthesized, characterized, and applied for the removal of cadmium ions from aqueous solutions. The adsorbent was prepared by combining chitosan, obtained from shrimp shells, with activated carbon derived from date pits, and zinc oxide nanoparticles, forming composite beads. The materials were characterized using FTIR, XRD, SEM-EDS, and BET analyses, which confirmed the successful synthesis of the bio-composite and revealed a rough, porous surface favorable for metal ion adsorption. Batch adsorption experiments were designed and optimized using Response Surface Methodology (RSM) with a Central Composite Design (CCD). Four process variables were investigated: initial Cd^{2+} concentration (C_0), adsorbent dosage (mads), solution pH, and temperature (T). Statistical analysis demonstrated an excellent fit of the quadratic model with R^2 = 99.87%, R^2(adj) = 99.70%, and R^2(pred) = 98.89%, confirming the reliability of the model. The response surface and contour plots highlighted significant interactions, particularly between pH and C_0, and between T and mads. Optimal operating conditions were found at pH = 6.86, mads = 0.05 g, C_0 = 300 mg/L, and T = 60 °C, yielding a maximum adsorption capacity of q = 27.41 mg/g with a global desirability of 1.0. Adsorption equilibrium was best described by the Freundlich and Redlich–Peterson isotherms, while kinetics followed the pseudo-second-order model. Moreover, the adsorbent exhibited high selectivity toward Cd^{2+} even in the presence of competing ions (Na^+, K^+, Mg^{2+}) and maintained strong reusability over five adsorption–desorption cycles, with only a slight decrease in efficiency from 83.76% to 80.18%.

Keywords: Cadmium removal, Bio-adsorbent, Chitosan–activated carbon/ZnO beads, Response surface methodology, Adsorption isotherms and kinetics, Water treatment

Recent Advances in Coordination Polymers for Wastewater Treatment

Malak Boussekine [1], Hamza Kherfi [1,2], Aouaouche Benkanoun[2]

[1]Laboratoire des Sciences Appliquées, Ecole National Supérieure des Technologies Avancées, Algiers, Algeria

[2] Laboratoire de Cristallographie-Thermodynamique, Faculté de Chimie, USTHB, BP 32 El Alia Bab Ezzouar, Algiers 16111, Algeria

Corresponding author: Malak Boussekine (ama.boussekine@ensta.edu.dz)

Abstract

Water is essential for life, and access to clean water is important for all living organisms. However, the constant presence of organic and inorganic pollutants in aquatic environments poses real threats to ecosystems and human health, requiring the development of effective and sustainable degradation technologies [1]. The emergence of innovative coordination polymers has taken water treatment to another level by offering alternatives to traditional materials for pollutants removal. This is due to their unique properties such as high surface area, ion exchange efficiency, and catalytic ability. Coordination polymers act as effective adsorbents and photocatalysts. Their adaptable structures and ability to produce highly reactive free radicals allow to target and break down pollutants such as antibiotics, heavy metals, and organic pollutants. For example, zinc-based coordination polymers have shown efficiency in photodegradation of organic dyes [2,3].In addition, coordination polymers are used in membrane technology for purifying water from salts and contaminants thanks to the high permeability and increased selectivity of the membranes formed by hybrid materials that combine organic polymers and coordination metal centers [4].In general, the use of coordination polymers in water treatment is very promising due to their high adjustability, versatility, and efficiency in removing contaminants. However, this does not mean that there are no challenges in their application, such as material stability, complexity of mechanisms, and economic feasibility [5].To facilitate their wider application, continuous progress is being made in the design of linkages, synthesis strategies, and mechanistic understanding in the development of next-generation coordination polymers for sustainable and efficient water treatment.

Keywords: Coordination polymers, Water treatment, Pollutant degradation.

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Green inhibitors from Carpobrotus acinaciformis leaves for carbon steel in acidic environments

Malika Khelfaoui [1, 2], Daoiya Zouied [1, 2], Karima Bekouche[1, 2]

1 LGCES Laboratory, Faculty of Technology, University of August 20, 1955, Skikda, Algeria

2 Department of Process Engineering, University of August 20, 1955, Skikda Algeria

Email : m.khelfaoui@univ-skikda.dz

Abstract

A major issue for both industry and society is industrial equipment corrosion, which seriously damages materials and equipment. This study investigates the application of leaf extracts from Carpobrotus acinaciformis (CA) as substitute corrosion inhibitors for C1020 carbon steel in hydrochloric acid (HCl). Two extraction techniques were used: methanolic extracts (CAM) and aqueous extracts (CAW) from the leaves of Carpobrotus acinaciformis. The extracts effectiveness in inhibiting corrosion was assessed using electrochemical characterization, which included polarization curves and electrochemical impedance spectroscopy (EIS). Chemical investigations revealed that when inhibitor concentrations grew, so did the inhibition efficiency (IE). At 350 ppm, the inhibitory efficiency (IE) of the CAM extract was 96.36%, whereas at 450 ppm, the CAW extract IE was 94.73%. According to the findings, CAM and CAW extracts can effectively and sustainably prevent corrosion in C1020 carbon steel in an acidic environment.

Keywords

Corrosion, carpobrotus acinaciformis, extraction, green inhibitor, impedance spectroscopy

Detoxification of Textile Dye Contaminated Wastewater Using Green Bioadsorbents

Marwa Bendaia [1,2]*, Sabir Hazourli [2], Naoual Houaidji [1], Sara Bennouar [1], Mohamed Bouziane[1]

[1] Materials Physico-Chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid - El Tarf University, P.B. 73, El Tarf 36000, Algeria.

[2]Département de Chimie, Laboratoire de Traitement des Eaux et Valorisation des Déchets Industriels, Faculté des Sciences, Université Badji –Mokhtar, Bp 12 Annaba 23000 (Algérie)

Email: m.bendaia@univ-eltarf.dz

Abstract

Water pollution by synthetic dyes represents a major environmental concern, particularly in the textile, cosmetic, and pharmaceutical industries. Among these dyes, Eriochrome Black T (EBT), a widely used anionic compound, is known for its toxicity and high resistance to biodegradation. To overcome the limitations of conventional treatment methods, adsorption has proven to be an effective, low-cost, and eco-friendly technique. In this study, bioadsorbents prepared from agricultural by-products, specifically eggshells (CO), were investigated for the removal of EBT from aqueous solutions. The adsorption performance was evaluated by examining the effects of several key parameters, including adsorbent dose, pH, ionic strength, and temperature. The results demonstrated that eggshells exhibit a significant adsorption capacity, confirming their potential as sustainable and low-cost materials for wastewater treatment. This work contributes to the valorization of agricultural waste while providing an environmentally friendly solution for the removal of synthetic dyes from industrial effluents.

Keywords: Dye, Biomass, Contamination, Treatment, Adsorption.

Elaboration and characterization physicochemical of copper oxide and their application in dye oxidation

Meriem Hamidani [1], Souad Djerad [2], Fadda Cherif [3]

Laboratory of Environmental Engineering, Department of Process Engineering, Badji Mokhtar-Annaba University, P.O. Box 12, 23000 Annaba, Algeria.

E-mail : meriem.hamidani@univ-annaba.dz

Abstract

Environmental pollution is one of the most critical and urgent problems of the world. Industries are the major polluters generating liquid effluents containing metals, dyes and other products that need to be treated. Approximately 10-15 % dyes are released into the environment making the effluent highly colored. In the last decades the decrease in rainfall is observed while water demand is in a constant increase. This situation makes the world's population facing major water crises. This problem constitutes a major challenge for researchers who tried to develop cost-effective technologies for wastewater treatment. In this study, copper was prepared with sodium ascorbate, an eco-friendly reagent. Micron sized particles were formed and mainly composed of metallic copper Cu with minor presence of Cu_2O. The product obtained was used in the oxidation of a dye (methyl orange) by an advanced Fenton-type oxidation process in which H_2O_2 was produced in situ. Different operating conditions were applied such as the effect of the mass of the copper, the temperature and the pH. The discoloration is complete after 40 min with 0.04 g of copper and at 60 ° C. Ultrasound was then applied at 60 °C in an acid medium in the presence of copper and the results was compared with those obtained with copper alone. The results show an improvement in the discoloration speed in the presence of ultrasound rapidly reaching 91.90% after 24 min compared with 77.46% in the presence of copper alone after the same reaction time.

Keywords: Ascorbate, Copper, Dye oxidation, Green process, Fenton-like.

Green Nanoparticle Synthesis for Vector Management: Sustainable Strategies Targeting Medically and Veterinarily Important Insects with a Focus on Diptera Culicidae

Mouna Cherairia [1], Samia Benrabah[2], Nedjoua Cheghib [3], Awatif Boumaza [1] & Amira Larafa [1,4]

[1] Department of Biology, University 8Mai 1945 Guelma, Guelma, Algeria
[2] Department of Geology, Geology Research Laboratory, Badji Mokhtar Annaba University, Annaba, Algeria
[3]Department of Material Sciences, Applied chemistry Laboratory, University 8Mai 1945, Guelma, Algeria
[4] Department of Biology, Laboratory of Biology, Water and Environment, University 8Mai 1945 Guelma, Guelma, Algeria

Corresponding author: Mouna Cherairia (monachairi@yahoo.fr)

Abstract

Animals and humans are increasingly vulnerable to various diseases, particularly parasitic infections transmitted directly or through insect vectors. Mosquitoes (Diptera: Culicidae) are of major medical and veterinary significance, acting as vectors for a wide range of pathogens, including protozoa, viruses, bacteria, and nematodes. Diseases such as malaria (transmitted by Anopheles), filariasis, yellow fever, dengue fever, Japanese encephalitis in humans, as well as bovine malaria and brucellosis in animals, continue to pose serious health challenges. These risks are further amplified by climate change, which fosters the expansion and proliferation of mosquito populations. To address these challenges, several vector control strategies have been adopted, including chemical insecticides and plant-derived compounds. However, increased concerns regarding environmental toxicity and the rapid emergence of insecticide resistance have encouraged the exploration of innovative, ecofriendly alternatives. In this context, **nanomaterial particularly green synthesized bionanoparticles, have emerged as a promising field,** offering new avenues for the sustainable control of mosquito vectors such as Culex species. Green synthesized nanoparticles exhibit potent larvicidal activity by inducing mortality and disrupting larval development at low, environmentally safe concentrations. As functional nanomaterials, they can be engineered to ensure controlled insecticide release by adhering to the larval cuticle or being ingested, enabling slow and targeted delivery of active molecules. This enhances larvicidal efficiency while minimizing ecological impact on aquatic environments. The integration of nanomaterial-based, ecofriendly strategies represents a sustainable and effective approach to Culex mosquito larval control. These methods reduce the limitations associated with conventional chemical insecticides, protect aquatic ecosystems, and support long-term sustainability in vector management programs aimed at reducing mosquito-borne diseases affecting both humans and animals.

Keywords: Green nanotechnology, Bionanoparticles, Biosynthesis, Insecticide resistance, Ecofriendly vector control.

Waste water sludge stabilization by chemical and electrochemical methods

Mouna Cherifi [1], Wahiba Mecibah[2], Sabir Hazourli [1]

[2]Département de Chimie, Université Badji-Mokhtar, Annaba/Laboratoire de Traitement des Eaux et Valorisation des Déchets Industriels
[2]Département de Technologie, Faculté de Technologie, Université 20 Août 1955 – Skikda, Algérie/ Laboratoire de Traitement des Eaux et Valorisation des Déchets Industriels
cherifimim@gmail.com

Résumé

Municipal and industrial wastewater treatment plants produce large amounts of sludge. It consists of high rates of organic, chemical and microbial pollutants. If they are not stabilized completely and discharged safely, they may become a potential pollution source, threatening soil and water bodies. This study comparatively investigated the disintegration of sewage sludge received from an urban wastewater treatment by peroxide hydrogen (H_2O_2) oxidation and an electrocoagulation process. H_20_2 oxidation pretreatment was optimized by the study of the effects of H_2O_2 dosage and the initial sludge pH-H_2O_2. The Batch EC experiments were carried out using aluminum, iron and zinc electrodes to investigate effect of treatment period, current density and pH. Sludge disintegration efficiency was studied in terms of solubilzation of sludge (SCOD), disintegration degree (DD), reduction of total solids (TS) and enhancement of sludge setteleability (SVI). The sludge disintegration data were utilized to compare the efficiency of various operational parameters. Finally, specific energy consumption was also discussed to determine the best operating conditions of EC process.

Keywords: sewage sludge, stabilization, chemical oxidation, electroccoagulation

Study on the treatment of wastewater and solid waste (sludge)

Anissa Necib[1], Rabiaa Djeribi[2], Boudjemaa Boughrara[3],

[1]Process engineering department, laboratory of chemistry of materials, university chadli benjedid, El Tarf, Algeria
[2] Process engineering department, laboratory of chemistry of materials, university; chadli benjedid, El Tarf, Algeria
[3] Chemistry department, laboratory of chemistry of material university chadli benjedid; El Tarf, Algeria
Necib anissa a.necib@univ-eltarf.dz

Abstract

Wastewater is collected and then sent to treatment plants where it is treated. At the end of the treatment and on leaving the station, the purified water is discharged into the natural environment; residual sludge, which is composed of water and dry matter containing mineral and organic substances, is collected and dried in the open air in specific beds. Residual sludge is above all a raw material composed of different elements (organic matter, fertilizing elements (N and P, etc.), metallic trace elements, organic trace elements and pathogens). The assessment of the quality of the sludge is based on the measurement of the physicochemical and chemical parameters, the chemical and mineral composition as well as on the presence or absence of organisms and aquatic microorganisms. Their final destination (agricultural, incineration, etc.)

Keywords: wastewater, physico-chemical quality, treatment plant, sludge

Lutte Contre L'eutrophisation Des Milieux Récepteurs Par L'élimination Des Nutriments (les phosphates et les nitrates) D'une Eau Usée Urbaine

Nawel Nedjah [1], Aicha Touhami [2], Mounir Nessaib[2]

[1]Université Alger 1, Laboratoire de métallurgie physique et propriétés des matériaux, Université Badji Mokhtar - Annaba, Algérie

[2]Ecole Nationale Supérieure de Technologie et d'Ingénierie,23005-Annaba

Corresponding author: Nedjah Nawel (nedjah23nawel@gmail.com)

Abstract

Pour remédier au problème d'eutrophisation il faut réduire la quantité d'azote et de phosphore rejetée dans les milieux récepteurs, c'est le but principal de notre travail de recherche. Nous avons opéré de façon à procéder à une élimination des phosphates et des nitrates physico-chimique et biologique d'une eau usée urbaine. Ce traitement combiné est basé sur la recherche de la dose optimale des différents coagulants choisi. Notre plan de travail est divisé en deux parties, la première étudie le traitement chimique par utilisation : la chaux, le chlorure ferrique et le sulfate d'aluminium comme coagulants pour ce traitement, tandis que la deuxième partie s'est intéressée à l'application du procédé par boues activées comme traitement biologique des eaux usées urbaines. Nous avons trouvé un bon rendement épuratoire en matière organique d'une valeur en DCO de 95% et en phosphore une valeur de 88%, pour le traitement chimique, et une valeur de 60% en DCO et 49% en phosphore dans le cas du traitement biologique

Keywords : Eutrophisation, azote, phosphates, coagulants, milieu récepteurs.

Analysis of Surface Water Quality in the Northeastern Region of Algeria

Hemza Ouaret [1], Tahani Derradji [1], Wafa Djemil[1], Mohamed Djidel[2]

1 University 8 May 1945 Guelma, Algeria

2 Kasdi Merbah University Ouargla, Laboratory of Sahara Geology, BP 511, 30000 Ouargla, Algeria

Corresponding author: Hemza OUARET (ouarethemza@gmail.com)

Abstract

In Algeria, water resources are limited and have been under increasing pressure due to population growth and the expansion of economic activities, leading to a growing demand. The studied region represents an important natural reservoir of surface and groundwater, where water serves as a key factor for socio-economic development. However, this dynamic has also generated negative impacts on water quality, affecting public health, soils, vegetation, and industrial activities. The objective of this study is to analyze the quality of surface waters in order to characterize their seasonal variations and identify the main influencing factors. The research approach includes the assessment of topographic, hydroclimatic, and lithological conditions, along with physico-chemical analyses, the calculation of calco-carbonic balance indices, and the application of water classification methods. The results indicate that the waters generally exhibit good chemical quality for agricultural (irrigation) and industrial uses. Nevertheless, continuous monitoring is recommended, particularly for potential use as drinking water, which may require additional treatment.

Keywords: Potability – Salinity – Aggressiveness – Corrosiveness – Water quality.

Etude de Phénomène d'Entartrage des Canalisations des Eaux Potables

Rabiaa Djeribi[1], Anissa Necib[2]

[1, 2] Process Engineering Department, Faculty of Science and Technology, Chadli Bendjedid University

Laboratory of Physical Chemistry of Materials (LPCM)

BP 73, ElTarf 36000, Algeria

djeribirabiaa4@gmail.com

Résumé :

L'eau est la plus importante pour l'existence de l'homme. Tous les circuits alimentés par des eaux sont confrontés au problème de formation de dépôt calco-carbonique au niveau des parois en contact avec l'eau. L'objectif de mon travail est d'évaluer la qualité physico-chimique des eaux (pH, turbidité, T, Cl^-, salinité, TH, TAC et MO) par une comparaison des échantillons en amont (station) avec des échantillons en aval (chez l'abonné), qui sont généralement la cause de phénomène d'entartrage dans les circuits de distribution d'eau potable. Pour une analyse courte du mois d'avril de tous les paramètres physico-chimiques de l'amont (station) en aval (chez l'abonné), on observe que les valeurs trouvées en amont et en aval sont pratiquement identiques et respectes les normes de potabilité algériennes et situe également dans les intervalles un proche aux normes de potabilisation dictée par l'Organisation Mondiale de Santé (OMS).

Mots clés : Eau, Entartrage, Caractéristiques physico-chimiques, pH, T, TH, TAC, MO.

Assessing the Physico-Chemical Quality of FERTIAL Annaba's Industrial Wastewater

Rania Necib [1], Soumeya Khaled-khodja [1], Abdenabi Abidi [2], Boudjema Boughrara[2], Rahma Boutaba [2]

[1]Science and Technology Faculty, Materials Physico-chemistry Laboratory, Chadli Bendjedid - El Tarf University, P.B. 73, El Tarf 36000, Algeria.
[2]Department of Process Engineering, Laboratory of Organic Synthesis, Modelling and Optimization of Chemical Process, University of Badji-Mokhtar, Annaba, 23000, Algeria
Rania Necib (r.necib@univ-eltarf.dz)

Abstract

An adequate supply of good-quality water is essential for the continuous development of any society. The most recent data on gross water use shows that total water withdrawals are steadily increasing. Uncertainties about the future of water resources amplify this challenge due to extreme weather events and climate change, increased competition for access to limited global water resources, and rising demand for better control of wastewater pollution to ensure more sustainable use of receiving waters. In the eastern region of Algeria, industrial activities are expanding, and their waste is released into the sea without proper treatment. Located 4 km from the city of Annaba, the Fertial group remains one of the industries whose discharges pose a major threat to the environment. The pollutants they release accumulate along the coast, affecting water quality and aquatic life, which can serve as biological indicators of pollution. The liquid effluents from the complex are problematic because they are released into coastal waters without prior treatment. In this study, we focused on evaluating the physicochemical quality of the wastewater originating from the complex. Parameters monitored included pH, temperature, BOD_5, COD, TSS, and nitrogen- and phosphorus-based compounds. The absence of treatment for these discharges may cause a high risk of eutrophication. Our analysis revealed an inferior quality of the wastewater, significantly exceeding national and international industrial discharge standards. Principal Component Analysis helped identify the pollutants that contribute most to the pollution of coastal waters.

Keywords: Physico-chemical quality, Industrial effluents, Wastewater, Fertial complex, Principal component Analysis, Eutrophication.

Development of a TBP-Based Electrochemical Sensor for the Detection of Bisphenol A

Selma Laguel [1], Mohamed elhadi Samar [2]

[1,2] Laboratory of Environmental Engineering, Department of Process Engineering, Faculty of Technology, Badji Mokhtar – Annaba University, P.O. Box 12, 23000 Annaba, Algeria.

selma.laguel@univ-annaba.dz

Abstract

The performance of a chemical sensor is governed by the synergistic adaptation between a selective receptor membrane and a physical transducer. This work presents a highly sensitive electrochemical sensor for detecting the endocrine disruptor Bisphenol A (BPA). The sensor is based on a selective polymeric membrane, incorporating Tri-butyl Phosphate (TBP) as an ionophore within a Siloprene K1000 matrix. Characterized by electrochemical impedance spectroscopy (EIS), the sensor was optimized for parameters such as TBP mass, immersion time, and pH. The optimized device achieved a wide linear detection range from 10^{-3} to 10^{-10} ppm, with an ultra-low detection limit of 10^{-10} ppm. The impedance response was accurately modeled using an equivalent circuit, validating the sensing mechanism. This TBP-based sensor demonstrates great potential for the monitoring of trace-level BPA in aqueous environments.

Keywords: Electrochemical sensor, impedance, TBP, Bisphenol A.

Caractérisation hydrochimique des eaux souterraines de la région de ben Yahia Abderrahmane dans la wilaya de Mila (Algérie)

Mounira Touati [1], Samia Benrabah[2]

[1]Department of Geology, Geodynamics and Natural Resources Laboratory (LGRN), Badji Mokhtar University, P.O. Box 12, Annaba 23000. Touati.mounira24@gmail.com.

[2]Department of Geology, Badji Mokhtar University, P.O. Box 12, Annaba 23000.Algeria

Abstract

This study assesses the lithological influence on groundwater chemistry in the Tamalous–Bin El Ouiden plain, located in northeastern Algeria. A total of 21 groundwater samples were collected and analyzed for physico-chemical parameters such as temperature, pH, and electrical conductivity, as well as the concentrations of major cations and anions. The objective is to characterize hydrochemical facies and identify geochemical processes controlling water composition. Analysis using Piper, Schoeller, and Stabler diagrams reveals a predominance of calcium-magnesium bicarbonate facies, with sodium-chloride facies also present in certain zones. The results indicate a relatively high level of mineralization, often linked to interactions between groundwater and local carbonate and evaporite geological formations. Data interpretation also suggests anthropogenic contributions in some areas. Comparison with World Health Organization (WHO) standards shows that most water samples are potable, although some exceed recommended thresholds, particularly for chloride and sodium. This work provides valuable insight into the chemical behavior of groundwater in a region experiencing both natural and human pressures, and highlights the importance of monitoring and sustainable management of water resources.

keywords: Groundwater chemistry, lithological influence, hydrochemical facies, geochemical interactions

Influence De La Modification De Surface Des Coquilles d'Amande Sur Les Propriétés Cinétiques Et La Capacité d'Adsorption Du Méthyle Violet

Wahiba Mecibah [1*], Mouna Cherifi [2], Nabila Boutemine[2], Souad Bouasla[3]

[1]Département de Technologie, Faculté de Technologie, Université 20 Août 1955 – Skikda, Algérie/ Laboratoire de Traitement des Eaux et Valorisation des Déchets Industriels
[2]Département de Chimie, Université Badji-Mokhtar, Annaba/Laboratoire de Traitement des Eaux et Valorisation des Déchets Industriels
[3]Université Ferhat Abas, Sétif-1, Algérie/Laboratoire d'ingénierie des matériaux et énergie, Faculté de Technologie, Université 20 Août 1955, Skikda, Algérie.

Mecibahwahiba@yahoo.fr

Abstract

L'objectif de ce travail est de comparer les performances des coquilles d'amande brutes (CAB) et modifiées (CAM) pour l'adsorption du colorant Méthyle Violet (MV), en se concentrant sur les gains d'efficacité massique et cinétique apportés par la modification. Bien que les deux matériaux atteignent des rendements maximaux comparables en milieu basique, les résultats mettent en évidence une amélioration significative de la cinétique et de l'efficacité massique pour le CAM. Le CAM atteint un rendement de 88.21% en seulement 60 minutes et avec une masse de 0.2 g, comparativement aux 100 minutes et à la masse de 1g nécessaires pour le CAB. Cette différence, en faveur du matériau modifié, suggère une augmentation de la surface active ou une meilleure accessibilité des sites d'adsorption, ouvrant la voie à l'utilisation de plus petites quantités de biosorbant pour une application industrielle.

Mots-clés : Biosorbant, Modification de surface, Adsorption, Cinétique, Coquilles d'amande.

Effect of pH in the detection of lead in aqueous medium

Riadh Zouaoui*[1,2], Saifi Issaadi[1,2], Mohamed Fahim Haroun [1,3]

1.2. Laboratory for electrochemistry of molecular and complex materials, Faculty of Science, Department of Chemistry, University Setif 1 Ferhat ABBAS, Algeria

1.3 Faculty of Science, Department of Chemistry, University Setif 1 Ferhat ABBAS, Algeria

* riadh.zouaoui@univ-setif.dz Tél: +213.662.65.49.77

Abstract

Buffer solutions have been widely used as supporting electrolytes for detection, due to their ability to fix the pH value and ionic strength. The pH value of a buffer solution exerts a significant but predictable effect on the preconcentration process. In this work we show the effect of pH on the peak current intensity of lead ion Pb^{2+} detection in different acetate buffer solutions of pH.

Keywords: electrochemistry, lead, peak intensity.

Effect of Concentration and pH on the Photocatalytic Degradation of Methylene Blue Using Mixed Oxide Catalysts

ADJOU Ouiza[1], IKKOUR Kahina[1], SELLAM Djamila[2], AITOUCHE Dounia[1]

1University of Bejaia, Faculty of Exact Sciences, Laboratory of Physico-Chemistry of Materials and Catalysis (LPCMC), 06000 Bejaia, Algeria.

2 Laboratory of Applied Chemistry and Chemical Engineering (LCAGC), Mouloud Mammeri University of Tizi-Ouzou (UMMTO), 15000 Tizi-Ouzou, Algeria.

Email: ouiza.adjou@univ-bejaia.dz

Abstract

The photocatalytic degradation of organic dyes such as methylene blue (MB) has received considerable attention due to their environmental persistence and use as model pollutants in photocatalytic studies. This work investigates the influence of key operational parameters— specifically the initial dye concentration and solution pH— on the visible-light-driven degradation of MB using mixed oxide photocatalysts. The catalysts were synthesized via an autocombustion method and characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller surface area analysis (BET), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and UV–visible diffuse reflectance spectroscopy (DRS). These analyses provided detailed insights into the structural, surface, and optical properties that determine their photocatalytic performance. Photocatalytic experiments revealed that increasing MB concentration led to a decline in degradation efficiency, mainly due to light attenuation and the saturation of active sites on the catalyst surface. In contrast, the solution pH exerted a strong influence on degradation kinetics, with optimal activity obtained under mildly basic conditions. This enhancement is attributed to improved dye adsorption and the greater availability of reactive oxygen species. Overall, the findings demonstrate that both dye concentration and pH critically affect photocatalytic behavior, offering valuable guidance for optimizing mixed oxide systems in wastewater treatment and environmental remediation applications.

Keywords: Photocatalysis; Methylene blue; Mixed oxides; Concentration; pH; Visible light; Water treatment.

ZnO–Based Mixed Oxides as Efficient Visible-Light Photocatalysts for the Degradation of Organic Pollutants

ADJOU Ouiza[1], IKKOUR Kahina[1], SELLAM Djamila[2], AITOUCHE Dounia[1]

[1]University of Bejaia, Faculty of Exact Sciences, Laboratory of Physico-Chemistry of Materials and Catalysis (LPCMC), 06000 Bejaia, Algeria.
[2] Laboratory of Applied Chemistry and Chemical Engineering (LCAGC), Mouloud Mammeri University of Tizi-Ouzou (UMMTO), 15000 Tizi-Ouzou, Algeria.
Email : ouiza.adjou@univ-bejaia.dz

Abstract

The increasing presence of persistent organic pollutants in aquatic systems has become a major environmental and health concern worldwide. Visible-light-driven photocatalysis represents an emerging and sustainable technology for the degradation of such contaminants, offering an energy-efficient and environmentally friendly alternative to conventional treatment methods. In this study, ZnO–based mixed oxide photocatalysts were synthesized via an autocombustion route and evaluated for their performance in the visible-light degradation of organic pollutants. Structural and optical characterizations were conducted using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), UV–visible diffuse reflectance spectroscopy (DRS) to examine crystallinity, surface morphology, and light absorption behavior. The introduction of secondary oxides into the ZnO matrix significantly enhanced visible-light absorption and improved photocatalytic efficiency compared to pure ZnO. These improvements are mainly attributed to the formation of heterojunctions, which promote efficient charge separation and suppress electron–hole recombination. Photocatalytic experiments using model organic compounds confirmed that the optimized mixed oxides exhibit superior degradation activity and stability under visible light. Overall, this study highlights the potential of ZnO–based mixed oxides synthesized by autocombustion as efficient and cost-effective photocatalysts for sustainable water purification and environmental remediation applications.

Keywords: ZnO–based mixed oxides; Visible light; Photocatalysis; Organic pollutants; Autocombustion; Water purification.

Investigation of the Inhibitory Effects of Natural UM and EJ Extracts Against Acid-Induced Corrosion

BEKOUCHE Karima[1], ZOUIED Daoiya[1,2]

[1]Department of Process Engineering, Faculty of Technology, University 20 August 1955 Skikda, 21000, Algeria

[2] Laboratory of Chemical Engineering and Environment of Skikda (LGCES) E-mail: krmbekouche21@yahoo.com

Abstract

The primary objective of this study is to enhance the anti-corrossion performance of extracts from EJ and UM plant as environmentally friendly corrosion inhibitors. The extraction of bioactive compounds from both plants was carried out using the Soxhlet extraction method, with ethanol serving as the extraction solvent. The inhibitory impacts of these extracts on the corrosion behavior of A106/B carbon steel in a 1 M hydrochloric acid (HCl) solution were evaluated using the mass loss method. The study also examined the influence of key operational parameters, including extract concentration, temperature, and immersion time, to determine their effects on the inhibition performance. Fourier Transform Infrared (FTIR) spectroscopy analysis revealed that both extracts contain a large number of organic compounds that are believed to be responsible for the inhibitory action. Experimental results demonstrated that the UM extract achieved a high inhibition efficiency, exceeding 90%, at a concentration of 400 ppm, a temperature of 298 K, and an immersion period of 4 hours. In comparison, the EJ extract also exhibited notable performance, with inhibition efficiencies ranging between 80% and 90% under the same conditions. Both UM and EJ extract can therefore be considered an optimal ecological inhibitors for protecting metals in acidic environments, providing a sustainable alternative to conventional chemical inhibitors.

Key words: Extracts, Corrosion, Inhibitor, HCl, Metal,

Influence De Zncl2 Sur La Corrosion De L'acier C-1020 Utilisé Comme Bac De Stockage

HOUIENE Zahia[1, 2], MARSA Zoubida[1, 3], RAMDANE Nassima[1, 3], MEDJANI Med Amine[1]

[1]Department of Chemistry, Faculty of Sciences, P.B 26, University of august 20, 1955 Skikda, Algeria [2]Ecocompatible Asymmetric Catalysis Laboratory (LCAE) Badji Mokhtar Annaba-University, B.P 12, 23000 Annaba, Algeria.
[3]Research laboratory LGCE, P.B 26, University of august 20, 1955, Skikda, Algeria

Corresponding author: zhouiene@yahoo.fr

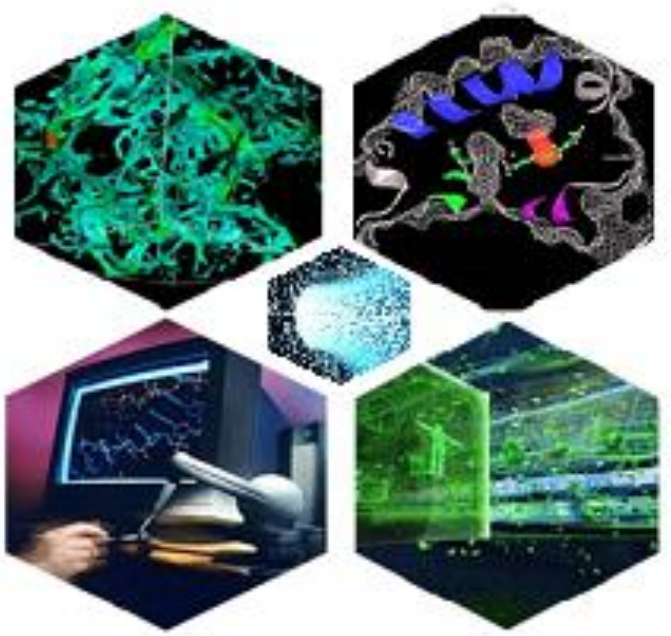
Résumé

La corrosion est le processus par lequel un matériau tend, sous l'effet d'un milieu agressif, à retourner à son état originel d'oxyde. Cette dégradation des matériaux, la prévention et la protection causent des pertes économiques considérables. Afin de lutter contre ce phénomène, l'objectif de ce travail, nous avons étudié l'évaluation de l'efficacité inhibitrice du chlorure de zinc contre la corrosion de l'acier C-1020 (réservoir de stockage) à pH différents (acide, neutre et basique) dans un milieu de chlorure de sodium (NaCl) de 10^{-2} M, en utilisant la méthode gravimétrique basée sur la perte de masse ainsi que la détermination des concentrations optimales. Les résultats obtenus montrent une bonne efficacité inhibitrice de $ZnCl_2$ à des pH neutres et basiques (EI% > 60%) en comparaison à ce trouvés dans le milieu acide (pH=5).

Mots clés : Corrosion, inhibiteur de corrosion, $ZnCl_2$, gravimétrie, acier.

Theme 4 :

Materials, Nanomaterials, Hybrid Materials, and Polymers



Geochemical Analysis of The Jebel-Onk Phosphate Deposit (Bir El Ater Area) Insights for Selective Exploitation and Resource Management

Salim Boulemia[1-2], Rihab Hadji[3-4], Rahal Abid[5]

[1] Faculty of Natural and Life Sciences Earth and the Universe, University May 8, 1945, Guelma, Algeria.

[2] Laboratory of sedimentary environment and hydric and minerals resources. Echahid Larbi Tebessi University, Tebessa, Algeria.

[3] Department of Earth Sciences, Institute of Architecture and Earth Sciences, Farhat Abbas University, Setif, Algeria.

[4] Laboratory of Applied Research in Engineering Geology, Geotechnics, Water Sciences, and Environment, Farhat Abbas University, Setif, Algeria.

[5] SOMIPHOS Company, P3R7+VRR, Bir El Ater, ZHUN II BP 122, Tébessa, Algeria.

ABSTRACT

This study focuses on the Jebel-Onk phosphate deposit to comprehend its geochemical characteristics and diverse phosphate facies. The various rock components from the Jebel-Onk deposit were identified. The investigation employed a method integrating geochemical data and lithological succession from core drilling to discern the phosphate deposit's morphology and the surrounding area, characterizing chemical element behavior simultaneously. The adopted method included automatic mapping of the Paleo-Eocene stratiform phosphate body, revealing spatial irregularities in thickness and establishing a correlation with the overlying supra-layer cover, comprising Ypresian and Lutetian flint limestones and Miocene sands. Results indicated fluctuations in chemical element contents for the two predominant phosphate types, beige and dark gray. Isotener maps highlighted spatial distributions, unveiling geochemical heterogeneities within the phosphate layer. Bi-variable statistical treatments elucidated correlation coefficients, showcasing a robust positive correlation between P_2O_5, CaO, and SiO_2, while revealing a negative correlation with MgO. Discussion, based on PCA, identified three distinct geochemical associations representing the phosphate material, the organic and dolomitic matrix, and the clay material. These findings offer valuable insights for guiding the selective exploitation of phosphates, facilitating efficient and informed resource utilization strategies.

Key words: Phosphate Deposit; Geochemical Data; Lithological Succession; Spatial Irregularities

Thermal and Kinetic Study of Metastable Phases in Al–Mg–Si Alloy

Alloui Fares

Laboratory LM2S, Badji Mokhtar University Annaba, Algeria

Corresponding author: Alloui Fares

E-mail : fares-sanousa@hotmail.fr

Abstract:

This work investigates the thermal behavior and precipitation kinetics of metastable phases in an Al–Mg–Si alloy without silicon excess. Differential Scanning Calorimetry (DSC) and microhardness measurements were employed to clarify whether the main exothermic peak observed in the DSC curve corresponds to a convolution of β″ and β′ phases or to a single metastable phase transformation. Isoconversional approaches (Kissinger–Akahira–Sunose, Friedman, Arrhenius) were applied to determine activation energies. The activation energy (44–70 kJ·mol^{-1}) confirms that the β″ phase dominates the studied peak. Microhardness tests show a decrease beyond 260 °C, supporting the dissolution of β″ precipitates. This combined thermal–mechanical analysis refines the understanding of metastable phase behavior in Al–Mg–Si alloys.

Representative Curves:
- DSC Curve
- Kissinger Plot
- Microhardness vs Temperature

The isoconversional method and differential scanning calorimetry as devices for studying solid materials: a case study of an excess Al-Si-Mg alloy

A. Hannachi[1, 2], A. Triki[2], M. I. Daoudi[2, 3, *]

[(1)] Department of Physics, Faculty of Sciences, Badji Mokhtar University, BP 12, 23 000 Annaba, Algeria

[(2)] LM2S Laboratory, Faculty of Sciences, Badji Mokhtar University, BP 12, 23 000 Annaba, Algeria

[(3)] Department of Mathematics and Computer Science, Faculty of Mathematics and Computer Science, University of 8 May 1945, 24 000 Guelma, Algeria,

*Correspondent author e-mail: daoudi.mourad@univ-guelma.dz, mourdaoudi@yahoo.com

Abstract

An Al-7Si-Mg casting alloy's microstructure and precipitation behaviors are the focus of this investigation. Following differential scanning calorimetry (DSC) investigations, the Avrami coefficients (n) and activation energies (E_α) are obtained. The Kissinger-Akahira-Sunose (KAS) method, which is an isoconversional approach, is employed to determine E_α which varies with the conversion α. The basis for calculating the coefficient n is the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation that describes the transformation kinetics. The obtained DSC curve shows the different peak transformations corresponding to β", β', Si, and β phases. The E_α values of these phases demonstrate that the diffusion of Si and Mg governs the mechanisms of their initial formation. However, the n values adequately explain the morphological transformations of these many phases. The transformation process of silicon receives special attention. It has been observed that the Si undergoes nanometric intra-dendritic α-Al precipitation, which, when continuously heated, takes the shape of rods and cobblestones. This evolution of the Si morphology, followed by Scanning Electron Microscopy (SEM) observations, was related to the obtained values of the Avrami coefficient.

Keywords: Cast Al-Si-Mg alloy, Differential Scanning Calorimetry, Kissinger-Akahira-Sunose (KAS) isoconversional method, nano-scale Si particles, rod-shaped Si particles

Biosynthesis and Characterisation of Iron Nanoparticles

Abderrahim Boutemedjet[1 2], Yehya Bouraghda[3 4]

[1]Department of Process Engineering, Laboratory of Physics for Matter and Radiation, University of Souk Ahras, Souk Ahras, Algeria
[2]Department of Process Engineering, Laboratory of Environmental Engineering, University of Badji Mokhtar, Annaba, Algeria.
[3]Department of Process Engineering, University of 8 Mai 1945, Guelma, Algeria
[4]Department of Process Engineering, University of Badji Mokhtar, Annaba, Algeria
Corresponding author :Abderrahim Boutemedjet (ab.boutemedjet@univ-soukahras.dz)

Abstract

The growing interest in green nanotechnology has led to the exploration of eco-friendly approaches for synthesising metallic nanoparticles with enhanced biocompatibility and functional properties.
In this study, iron nanoparticles (were synthesised via a biological route using plant extracts as natural reducing and stabilising agents. The biosynthetic method offers an alternative to conventional chemical and physical techniques by eliminating the need for toxic reagents and harsh conditions, thus ensuring environmental sustainability and cost efficiency.

The formation of FeNPs was visually indicated by a colour change during the reaction process. The obtained nanoparticles were characterised using X-ray Diffraction (XRD) and Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM–EDS). XRD analysis showed an amorphous structure of the synthesised iron nanoparticles, while SEM images revealed their morphology and particle size within the nanometre range. The EDS spectrum verified the elemental composition, confirming the presence of iron, with presence of biomolecules from the plant extract responsible for stabilisation.

The biosynthesised iron nanoparticles exhibit desirable physicochemical properties that make them promising candidates for environmental, biomedical, and catalytic applications. This study demonstrates that biological synthesis is an efficient, eco-friendly, and sustainable method for producing iron nanoparticles with controllable properties and potential for diverse scientific and industrial uses.

Keywords: Biosynthesis, Iron nanoparticles, Plant extract, X-ray diffraction (XRD); Scanning electron microscopy (SEM).

Structural, electronic and Thermodynamic properties of $KBeCl_3$ halide perovskites using FP-LAPW method

Imene Beldi [1], Nassima Chouit [2], Manouba Slimani [2], Hocine Meradji[2] and Sebti Ghemid[2]

[1] Laboratory LSC, Department of Physics, Badji Mokhtar University Annaba, Algeria.

[2] Laboratory LPR, Department of Physics, Badji Mokhtar University Annaba, Algeria.

Corresponding author: Beldi Imene

e-mail : beldi_imene@yahoo.fr

Abstract

This study presents a first-principles investigation of the perovskite compound $KBeCl_3$ using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method within the framework of Density Functional Theory (DFT). Structural optimization confirms the stability of the cubic perovskite phase. The calculated lattice parameters are in good agreement with theoretical expectations. Electronic band structure analysis reveals the semiconducting nature of $KBeCl_3$, with an indirect band gap. Thermodynamic properties such as the Debye temperature, specific heat, and thermal expansion coefficient are also evaluated. The material exhibits favorable stability at high temperatures. These findings suggest that $KBeCl_3$ could be a promising candidate for optoelectronic or thermoelectric applications. Overall, the study provides valuable insights into the fundamental properties of this halide perovskite.

Keywords: Debye model, Thermal properties, DFT, wien2k

Effect of Plasma Nitriding on Corrosion Resistance of AISI 2205 Stainless Steel

Selma Attabi [1], Majda Mokhtari[2]

[1]Department of Mechanical Engineering, Laboratory of Applied Mechanics of New Materials, University of 08 Mai 1945, Guelma, Algeria

[2]Department of Physics, University of Oum el bouaghi, Algeria

Corresponding author: Attabi Selma (attabi.selma@gmail.com)

Abstract

Duplex stainless steel is increasingly used as an alternative to traditional austenitic stainless steel, thanks to its high strength, adequate ductility, lower nickel content, and excellent corrosion resistance. These enhanced properties result from its dual-phase microstructure, combining both austenitic and ferritic phases. Since based AISI 2205 components are subjected to severe environments of high temperature, wear and corrosion, it is critical to improve their surface properties to prevent any premature failure. In this work, a surface treatment of plasma nitriding was applied on this stainless steel and its corrosion was studied through electrochemical tests. Microscopic observations showed the formation of thin nitrided layer (e=8,3 µm) due to the surface treatment. Based on the linear polarization curves, results indicated that treated surface showed both descreased corrosion potential E_{corr} and lower corrosion cuurent I_{corr} . The corrosion rate of nitrided sample was also five times much lower than the corrosion rate of non-treated surface.

Keywords: Nitriding, AISI 2205, corrosion.

Effect of sintering temperature on the properties of CuNi alloy

BRAHIMI Afef[1], KHADRAOUI Ahlem[1], HOUAIDJI Nawal[1], LOCIF Redouani[1]

[1] Materials Physico-Chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid - El Tarf University, P.B. 73, El Tarf 36000, Algeria.

Abstract

This work focuses on the study of some physical properties of the CuNi binary alloy prepared by high-energy mechanical milling at 5 h and sintered in a furnace at different temperatures with a two-hour holding time, followed by slow cooling in the furnace. Samples were analyzed by X-ray diffraction (XRD) in a Bruker D8 diffractometer and Vickers microhardness testing. The main objective is to understand the influence of the sintering temperature on the structural, microstructural, and mechanical properties of the product. The results reveal the formation of a solid solution Cu0.81Ni0.19 of CFC structure, the presence of oxides from 600°C, and the growth of microhardness with increasing sintering temperature.

Key words: alloy, mechanical grinding, XRD, Vickers microhardness test.

Mechanical Stability and Thermal Behavior of Na_2NbTaO_6: A First-Principles Study

Aissani Ali[3], Ouendadji Salima[1,2*], Fouad El Haj Hassan[4]

[1]Laboratoire des couches minces et interface Université Frères Mentouri Constantine 1 - BP, 325 Route Ain el Bey, 25017 Constantine Algeria

[2]Laboratoire de Physique des Rayonnements, Département de Physique, Faculté des Sciences, Université de Annaba, Algeria.

[3]Technology and Solids Properties Laboratory, Faculty of Science and Technology, University of Mostaganem (UMAB), Algeria

[4]Basic and Applied Sciences Research Center, Al Maaref University, Airport Avenue, Beirut, Lebanon

*Ouendadji.salima@umc.edu.dz

Abstract:

The mechanical behavior of the cubic double perovskite **Na_2NbTaO_6** was studied using first-principles calculations based on density functional theory. The results confirm that the compound is mechanically stable and possesses a compact and rigid lattice structure. Analysis of the elastic parameters indicates a brittle mechanical response with moderate anisotropy and partial covalent bonding. The estimated melting temperature and thermal indicators reveal strong resistance to heat and deformation, suggesting that **Na_2NbTaO_6** is suitable for applications requiring both mechanical strength and thermal reliability.

Keywords: Na_2NbTaO_6, mechanical properties, DFT, stability, thermal resistance

Title of the Paper: 2D BiXY (X≠Y) Monolayers For Hydrogen Evolution Reaction: A DFT Study

Akroud Karima[1], Benamara Ouarda[2], Zanat Kamel[3]

[1] Physics laboratory at Guelma, Faculty of Mathematics, Computing and Material Sciences, University 8 May 1945 Guelma, P.O. Box 401, Guelma 24000, Algeria

[2] Physics laboratory at Guelma, Faculty of Mathematics, Computing and Material Sciences, University 8 May 1945 Guelma, P.O. Box 401, Guelma 24000, Algeria

[3] Physics laboratory at Guelma, Faculty of Mathematics, Computing and Material Sciences, University 8 May 1945 Guelma, P.O. Box 401, Guelma 24000, Algeria

Corresponding author: Akroud Karima (akroud.karima@gmail.com)

Abstract

Two-dimensional BiXY monolayers (X≠Y) represent an emerging class of materials with intriguing properties for photocatalysis and energy applications. Our Density Functional Theory (DFT) calculations, carried out using the PBE functional, show that BiXY exhibits an indirect band gap. While the indirect nature may reduce transition probability compared to direct-gap systems, the material still absorbs efficiently in the visible-light region, allowing effective utilization of solar radiation. Crucially, the conduction band minimum (CBM) lies at a favorable energy level with respect to the hydrogen reduction potential, enabling the hydrogen evolution reaction (HER). This alignment suggests that BiXY monolayers can act as efficient photocatalysts for hydrogen production. Together with their electronic stability and light-harvesting capability, these findings position BiXY monolayers as attractive candidates for applications in **hydrogen generation, Energy Storage, and next-generation optoelectronic devices**.

Keywords: Monolayers, DFT, Photocatalysis, Hydrogen Evolution Reaction (HER), Energy Storage.

Effect of Chromium Doping Concentration on the Structural, Optical, and Electrical Properties of ZnO Thin Films for UV Photodetector Applications

Atef Chibani [1], Sara Benzitouni[2], Abdelhakim Mahdjoub[3], Amal Mezbache[2]

[1] Research Center in Industrial Technologies CRTI, P.O. Box 64, Cheraga 16014, Algiers, Algeria.

[2]Laboratory of Active Components and Materials, University Larbi Ben M'hidi Oum El Bouaghi, Oum El Bouaghi 04000, Algeria.

[3]Laboratory of Materials and Structure of Electromechanical Systems and Their Reliability, University Larbi Ben M'hidi Oum El Bouaghi, Oum El Bouaghi 04000, Algeria.

Corresponding author: Sara Benzitouni (Benzitouni.sara@gmail.com ; chibaniatef@gmail.com)

Abstract

The present study investigates the effect of chromium (Cr) doping concentration on the structural, morphological, optical, and electrical properties of ZnO thin films deposited on glass substrates. Structural characterization using X-ray diffraction (XRD) revealed that all films exhibit a polycrystalline hexagonal wurtzite-type structure, with the most intense diffraction peaks corresponding to the (002) and (103) planes at 34.42° and 63.63°, respectively. The decrease in lattice parameter c and crystallite size with increasing Cr concentration is attributed to the substitution of smaller Cr^{3+} ions (0.615 Å) for Zn^{2+} ions (0.74 Å), which also leads to an increase in dislocation density and a consequent deterioration of crystallinity. Atomic force microscopy (AFM) images show dense and rough film surfaces, with the average grain size decreasing from 140 nm to 7 nm as Cr concentration increases, followed by a slight increase to 20 nm, likely due to growth competition between ZnO and Cr_2O_3 phases. Optical studies indicate high transparency (60–85%) in the visible region (400–1100 nm), with transmittance decreasing upon doping. A blue shift in the absorption edge and an increase in optical band gap energy with Cr content are observed, which may result from lattice distortions and tail band formation. Electrical measurements show that resistivity increases with Cr doping, while carrier concentration and mobility remain nearly constant. Finally, the photodetection behavior of the films under UV illumination demonstrates their potential applicability as UV photodetectors.

Keywords: Cr- doping; ZnO thin films; AFM analysis; electrical properties; XRD; UV photodetector

Green Synthesis, of TiO_2 Nanoparticles Doped with Different Cu Concentrations using Portulaca Qleracea L. leaf extract and evaluation of their antibacterial activity

Mohammed Abdelkader Belalem [1], Mohammed Said Nedjimi [2], Belhabib Laouthar[2] and Bouhnik Seida Khadidja[2]

[1]Sciences and Environmental Research Laboratory, Department of Material Sciences, Faculty of sciences and technology, University of Tamanghasset, 11000 Tamanghasset, (Algeria)

[2]Faculty of Mathematics and Material Sciences, Department of Chemistry, University of Kasdi Merbah Ouargla, 30000 (Algeria)

Corresponding author: Mohammed Abdelkader Belalem: belalem1962@gmail.com

Abstract

This study achieved a significant scientific milestone by successfully synthesizing copper- doped titanium dioxide nanoparticles (TiO_2) through a green approach using purslane (Portulaca oleracea L.) extract. This method was distinguished by its environmental friendliness and cost-effectiveness compared to traditional chemical methods. The results demonstrated the high efficiency of the plant extract in reducing metal ions and stabilizing nanoparticles, attributed to its bioactive compounds such as flavonoids and amino acids.

Advanced characterization techniques, including UV-Vis spectroscopy and Fourier-transform infrared spectroscopy (FTIR), confirmed the successful synthesis and stability of the nanoparticles. Additionally, the nanoparticles exhibited significant antibacterial activity against strains such as Escherichia coli (E. coli) and Klebsiella pneumoniae (K. pneumoniae), opening promising avenues for medical and environmental applications.

These findings underscore the importance of adopting green synthesis methods for nanomaterials, which combine scientific efficiency with environmental sustainability, while also holding potential for scaling up in industrial and biomedical applications.

Keywords: Green synthesis, Titanium dioxide, Nanoparticles, Portulaca oleracea L., Antibacterial activity

Study of Tool Material Behaviour and Wear Mechanisms in Hard Turning of Hardened Steels

Bouchelaghem Hadjira[1], Gherdaoui Hamza[1], Rima Bouhali[2], Yallesse Mohamed Atman[1]

[1] Mechanical Engineering Dept, Mechanics and Structures Research Laboratory (LMS), Université 08 mai 1945, Guelma.24000, Algeria

[2] Higher Normal School of Technological Education ENSET Laboratory of Physical Chemistry and Biology of Materials, Skikda 21000, Algeria

Corresponding author: bouchelaghem.hadjira@univ-guelma.dz

Abstract

The present work falls within the field of **hard turning**, a modern machining process that tends to replace grinding for the finishing of **hardened steels**, due to its flexibility, economic efficiency, and ability to produce high-quality surfaces. The experimental study focuses on the hard turning of **high-alloy steel AISI D3**, heat-treated to a hardness of 60 HRC, a material well known for its high mechanical strength and machining difficulty. The main objective is to **compare the cutting performance of various tool materials,** namely **cubic boron nitride (CBN), alumina-based ceramics (CC6050, CC650, and CC670),** and the **coated carbide GC4005,** in order to evaluate their capability to withstand the severe conditions of hard turning. The analysis is based on two key criteria: **tool wear resistance** and its influence on **surface roughness**, which are decisive parameters in assessing process quality. Experiments were conducted at different cutting speeds to investigate the effect of this parameter on tool wear behaviour and surface quality. The results aim to identify the tool material offering the best compromise between tool life, dimensional stability, and surface finish, while contributing to a better understanding of wear mechanisms such as abrasion, diffusion, and oxidation. This work is therefore part of an overall effort to **optimize hard turning**, aiming to enhance performance, productivity, and process profitability while reducing the need for grinding and its environmental impact.

Keywords : Tournage dur, AISI D3, Usinabilité, Matériaux de coupe, Rugosité de surface, Mécanismes d'usure.

A Study of The Thermal and Structural Properties of a Copper-Based Alloy Produced by High-Frequency Melting Methods.

BOUTABBA Mohamed Ali[1], LAYACHI Fahima[2], DEBILI Mohamed Yacine[3]

[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA

[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA

[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA

Corresponding author: BOUTABBA Mohamed Ali (mouhamedali9623@gmail.com)

Abstract

This work involves the experimental characterisation of a ternary metallic alloy consisting of Cu-18%Al-2%Zn, which was obtained through high-frequency melting under magnetic induction. Regarding the solidification structure, optical microscopy (OM) revealed, by contrast difference after sample preparation, that the alloy has at least two different phases. The matrix of this alloy appears with a dendritic solidification front developed in secondary branches. X-ray diffraction (XRD) showed, moreover, that the microstructure of this ternary Copper alloy contains two different intermetallic compounds, which are Cu_3Zn_8 and the matrix $AlCu_3$. The differential scanning calorimetry (DSC) curve has finally confirmed the XRD results by showing two endothermic peaks, respectively at 572°C and 1053°C, related to the dissolution of the intermetallic Cu_3Zn_8 and melting of $AlCu_3$.

Keywords: Copper; OM; XRD; DSC; Phases.

Development And Microstructural Characterization of a Copper–Based Alloy Made by High Frequency Melting

BOUTABBA Mohamed Ali[1], LAYACHI Fahima[2], DEBILI Mohamed Yacine[3]

[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA
[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA
[1]Physics Department, LM2S Laboratory, Badji-Mokhtar University, ANNABA, ALGERIA

Corresponding author: BOUTABBA Mohamed Ali (mouhamedali9623@gmail.com)

Abstract

This work is an experimental study, and non-destructive characterization, of a ternary-based alloy Cu-28%Al-2%Zn obtained by high frequency (HF) melting under magnetic induction. The copper-aluminum-zinc alloy, here studied, was quenched from the liquid state to room temperature. With regard to the solidification structure, optical microscopy (OM) showed that the alloy has a microstructure with a dendritic solidification front developed in secondary branches. Scanning electron microscopy (SEM), in back scattered electron mode, revealed the presence of two phases with different chemical contrasts. X-ray diffraction (XRD) and differential scanning calorimetry (DSC) showed, moreover, that the microstructure of the ternary Cu-28%Al-2%Zn alloy contains not only three intermetallic compounds Cu_5Zn_8, $AlCu_3$ and Al_4Cu_9 but also the metastable phase Cu_3Zn which appears with an endothermic peak in the DSC measurement.

Keywords: Copper; HF melting; Alloys; characterization; Phases.

Structural, Optical and Mechanical Properties of Nichrome.

Naoual Houaidji[1, *], Wassila Tebib[1], Marwa Bendaia[1], Afef Brahimi[1], Ahlem Khadraoui[1]
[1] Materials Physico-Chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid - El Tarf University, P.B. 73, El Tarf 36000, Algeria.

Corresponding-author [*]: n.houaidji@univ-eltarf.dz

Abstract

Nanomaterials are solid materials made partially or totally of nano-objects whose size varies along a spectrum of nanometric dimensions. Ni-Cr based alloys have been known for a long time, are intensively studied and are used in many applications. A binary nickel-chromium alloy ($Ni_{67}Cr_{33}$) produced by high-energy grinding and sintering. The samples studied were produced by compressing the base powders under a 15T load and then sintered at 800°C for 3 hours. They were then cooled in a furnace. For characterization, several types of analyses were performed: X-ray diffraction (XRD), metallographic observation, and Vickers microhardness testing. The results of the analyses XRD revealed the existence of the $NiCr_2$ phase and the Ni(Cr) solid solution, which has a nanometric structure. Metallographic observation revealed some information about the microstructure of our samples, including the heterogeneity and dispersion of micropores as well as the existence of two different contrasts. The microhardness study highlights that the grinding time of 4 hours seems optimal to maximize hardness via structural refinement and efficient densification.

Key words: Ni-Cr alloys, mechanical alloying, sintering, X ray diffraction.

Analyse des Effets des Conditions de Coupe sur le Perçage des Composites Renforcés par Fibres de Verre

Frioui Nadia[1] Hamlaoui Nacira[2], Ahmed Belaadi[3] Messaouda Boumaaza[4]

[1]Mech. Eng. Dept., Université 8 Mai 1945 Guelma, P.O. Box 401, Guelma 24054, Algeria,

[2] Mech. Eng. Dept., Université 8 Mai 1945 Guelma, Mechanics of Materials & Plant Maintenance Research Lab (LR3MI), Mechanical Eng. Dept., Badji Mokhtar University, P.O. Box 12, Sidi Amar,23005 Annaba, Algeria.

[3]Département de génie mécanique, Faculté de Technologie, Université 20 août 1955 Skikda, Skikda, Algeria ; Laboratoire des Silicates, Polymères et Nanocomposites (LSPN), Université 08 Mai 1945, Guelma, Algeria

[4]Laboratoire de Génie Civil & Hydraulique (LGCH), Université 8 Mai 1945, Guelma, Algeria

Corresponding author: frioui.nadia@univ-guelma.dz

Résumé

Les matériaux composites renforcé de fibre de verre (GFRP) trouvent de plus en plus d'applications dans les secteurs industriels, l'automobile, l'aéronautique et de construction de vaisseaux spatiaux et les véhicules marins en raison de leurs avantages significatifs sur les autres matériaux. Ils offrent une résistance/rigidité spécifique élevée, une résistance supérieure à la corrosion, un poids léger, faible conductivité thermique, haute résistance à la fatigue, et résistance aux produits chimiques et attaques microbiologiques. En raison de l'élargissement de la gamme d'applications du GFRP, l'usinage de ces matériaux est devenu un sujet de recherche très important.

L'usinage des matériaux composites est une tâche complexe en raison de leur hétérogénéité, de leur anisotropie et de la forte abrasivité des fibres, et il présente des problèmes dans l'opération de perçage tels que le délaminage, arrachement des fibres, écaillage, dégradation thermique. La compréhension fine des paramètres de coupe constitue un enjeu majeur pour la maîtrise des phénomènes liés à l'usinage des composites. A cet effet des plans d'expérience ont été réalisés. Des modèles empiriques tirés de ces plans d'expériences permettent de prédire le délaminage en entrée et en sortie du trou. L'analyse Statique, a été introduite afin de déterminer l'impact des paramètres de coupes et leurs contributions.

Mots clés : GFRP, délaminage, Composite, Perçage

Structural And Electronic Properties of AlP: A DFT Study Using Wien2k

Guemmoud Nassima[1]

[1]Faculty of Science Department physic University Badji Mokhtar Annaba Algeria
Nassima.guemmoud@univ-annaba.dz
guemmoudnassima@gmail.com

Abstract

In this work, we report a structural and electronic propriety of aluminum phosphide (AlP), study of III-V binary semiconductors crystallizing in the zinc blende. Using the WIEN2K code based on density (DFT), with the generalized Gradient Approximation (GGA), (LDA) and (WC). The optimized lattice parameters are in good agreement with experimental data . The electronic band structure reveals the semiconducting behavior of AlP with an indirect band gap. As AlP is promising material for nanoscale electronic and optoelectronic devices, this work contributes to the broader understanding of its fundamental properties within the framework of Nanomaterials and Nanotechnology. The results may support future development of AlP based nanostructure for energy and photonic applications.

Keywords: AlP, WIEN2K, DFT, GGA, LDA, WC, electronic structure, band gap, nanomaterials.

Caractérisation Morphologique Et Chimique Des Fibres Naturelles De Spartium junceum L. Traitées Pour Le Renforcement Des Biopolymères

Hadjer Chelighem [1], Aida Benhamida[2]

[1,2] Département de Génie des Procédés, Laboratoire de silicates, polymères et nancomposites (LSPN), Université 8 Mai 1945 Guelma, Algérie
Corresponding author: Hadjer Chelighem, Aida Benhamida (chelighem.hadjer@univ-guelma.dz)

Résumé

L'étude de la morphologie et de la composition chimique des fibres végétales traitées est essentielle pour comprendre leur comportement dans les biocomposites. Dans ce travail, des fibres de Spartium junceum L., extraites manuellement puis soumises à des traitements alcalin (NaOH) et silanique (APTES), ont été caractérisées à l'aide d'analyses structurales et spectroscopiques. L'objectif est d'évaluer les effets de ces traitements sur la propreté de la surface, la structure chimique et la compatibilité interfaciale avec le polymère biodégradable PHBV. L'observation par microscopie électronique à balayage (MEB) a révélé une amélioration significative de la morphologie des fibres après traitement. Les surfaces deviennent plus rugueuses, exemptes d'impuretés et présentent des fibrilles plus exposées, favorisant ainsi l'ancrage mécanique avec la matrice polymère. Les analyses par spectroscopie infrarouge à transformée de Fourier (FTIR) ont montré une diminution notable des bandes caractéristiques de la lignine et des hémicelluloses, confirmant leur élimination partielle par le traitement alcalin. L'apparition de nouvelles bandes correspondant aux groupes silanols et siloxanes après greffage du silane confirme la modification chimique réussie de la surface fibreuse. Ces résultats démontrent que la combinaison des traitements alcalin et silanique conduit à une amélioration structurelle et chimique des fibres, leur conférant de meilleures propriétés d'adhésion et de compatibilité avec les polymères biodégradables. Ce travail ouvre la voie à l'élaboration de biocomposites renforcés performants à base de Spartium junceum, contribuant à la valorisation de la biomasse végétale locale dans une optique de développement durable.

Mots clés : Spartium junceum, MEB, FTIR, Traitement alcalin, Silane, Compatibilité, PHBV, Biocomposite

Extraction Et Traitement Des Fibres Végétales Naturelles Pour Le Renforcement Des Biocomposites

Hadjer Chelighem [1], Aida Benhamida[2]

[1,2] Département de Génie des Procédés, Laboratoire de silicates, polymères et nancomposites (LSPN), Université 8 Mai 1945 Guelma, Algérie
Corresponding author: Hadjer Chelighem, Aida Benhamida (chelighem.hadjer@univ-guelma.dz)

Résumé

Dans le cadre du développement de matériaux durables issus de ressources renouvelables, les fibres végétales naturelles constituent des renforts prometteurs pour les polymères biodégradables. L'objectif principal de ce travail est d'extraire et de traiter les fibres longues issues du Spartium junceum, une plante locale abondante en Algérie. L'extraction a été réalisée manuellement après une étape de séchage et de défibrage mécanique afin d'obtenir des fibres continues de bonne qualité. Par la suite, des traitements chimiques ont été appliqués dans le but d'améliorer la propreté de la surface et la compatibilité avec la matrice polymère. Le traitement alcalin à la soude (NaOH) a permis d'éliminer partiellement les constituants amorphes tels que les hémicelluloses, la lignine et les cires, tout en augmentant la rugosité et la réactivité de la surface. Un second traitement, à base de silane (APTES), a ensuite été appliqué pour introduire des groupes fonctionnels capables d'assurer des liaisons chimiques entre la fibre et la matrice polymère biodégradable (PHBV). Ces modifications visent à renforcer l'adhésion interfaciale et à réduire les phénomènes de décollement observés dans les composites non traités. Les fibres traitées ont présenté un aspect plus propre, une texture plus rugueuse et une meilleure aptitude à l'imprégnation dans la matrice. Ce travail constitue une étape clé dans la valorisation des plantes locales en tant que source de fibres naturelles performantes, tout en s'inscrivant dans une approche écologique et éco-efficace pour la conception de biocomposites à faible impact environnemental.

Mots clés : Spartium junceum, Extraction manuelle, Traitement alcalin, Silane, Compatibilité, Biocomposites, PHBV.

Effet de l'Acide Chlorhydrique sur le Polyéthylène de haute densité

Hamlaoui Nacira[1,2], Frioui Nadia[3] Bouslah Kouka[4], Chaoui Kamel[2]

[1]Mech. Eng. Dept., Université 8 Mai 1945 Guelma, P.O. Box 401, Guelma 24054, Algeria,

[2]Mechanics of Materials & Plant Maintenance Research Lab (LR3MI), Mechanical Eng. Dept.,

Badji Mokhtar University, P.O. Box 12, Sidi Amar,23005 Annaba, Algeria.

[3)] Mech. Eng. Dept., Université 8 Mai 1945 Guelma, P.O. Box 401, Guelma 24054, Algeria.

[4)]LR3MI and LTSE, National Higher School of Technology and Engineering, Dept. Process Eng. & Energetics, 23005 Annaba,

Corresponding author: Hamlaoui Nacira (hamlaoui.nacira@univ-guelma.dz)

Résumé :

Les polymères sont des matériaux durables, mais généralement ils peuvent être exposés à des substances qui les détériorent, et se rompent de manière prématurée.

La durabilité des réseaux de conduites en polyéthylène de haute densité (HDPE) est un facteur important à prendre en compte dans l'estimation de la durée de vie. Cette durabilité participe à la réduction considérable des coûts de maintenance et de réhabilitation en fonction de la nature des matériaux utilisés.

Les agents chimiques comme les eaux savonneuses, quelque acides organique, les hydrocarbures aromatiques et halogènes affectent de manière adverse les thermoplastiques. L'objectif de cette étude est d'examiner influence de l'acide chlorhydrique HCL à trois différents pourcentages sur la résilience du tube en polyéthylène HDPE 100 à température ambiante. L'acide chlorhydrique à forte concentration attaque chimiquement le HDPE et provoque une augmentation de la résilience de l'ordre de 14,76%.

Mots clés : Polyéthylène, Tube HDPE-100, HCL, Résilience

Green Synthesis of Zinc Oxide Nanoparticles Using (Juniperus phoenicia) Extract and Evaluation of Their Antibacterial Efficacy

Hayat ZERROUKI[1], Mohammed Said NEDJIMI[1], Mohamed Lakhder BELFAR[1], Amina BELMEHDI[1]

[1]VPRS Laboratory, Faculty of Mathematics & Matter Sciences, University of Kasdi Merbah, B.P. 511, 30000, Ouargla, Algeria

Corresponding author: hayat zerrouki (zerroukih2020@gmail.com)

Abstract

This study successfully achieved the green synthesis of Zinc Oxide Nanoparticles (ZnO NPs) using an aqueous extract of the Juniperus phoenicea plant, presenting an eco-friendly alternative to conventional chemical methods. The synthesized nanoparticles were characterized using UV-Visible (UV-Vis) and Fourier Transform Infrared (FT-IR) spectroscopy. A distinct absorption peak at approximately 370 nm in the UV-Vis spectrum confirmed nanoparticles formation. FT-IR analysis identified functional groups from the plant extract, such as O-H, C=O, and C-O, on the nanoparticles surfaces, and a peak below 700 cm^{-1} verified the presence of Zn-O bonds. The antibacterial efficacy of the ZnO NPs was evaluated against three bacterial strains: Staphylococcus aureus, Escherichia coli, and Klebsiella. The results demonstrated significant, dose-dependent antibacterial activity. The highest concentration (0.2 mg/ml) was the most effective, with the largest inhibition zone observed against Staphylococcus aureus (1.9 cm), followed by Escherichia coli (1.2 cm) and Klebsiella (0.9 cm). In conclusion, this research confirms that Juniperus phoenicea extract is effective for the green synthesis of Zinc Oxide Nanoparticles, which exhibit promising antibacterial properties, highlighting the potential of this sustainable approach for biomedical applications.

Keywords: Green Synthesis, Zinc Oxide Nanoparticles, Juniperus phoenicea, Antibacterial Activity

Bio-Based and Environmentally Friendly Water Remediation Employing Chitosan from Edible Mushrooms

Imane Kouadri [1], Bachir Ben Seghir [2], Abdelkrim Rebiai [3], Abdelheq Layachi [4]

[1] Department of Process Engineering, Laboratory of Industrial Analysis and Materials Engineering (LAGIM), University May 8 1945, Guelma, Algeria
[2] Department of Process Engineering and Petrochemical, Laboratory of Renewable Energy Development unit in Arid Zones (UDERZA), University of El Oued, El Oued, Algeria
[3] Department of Process Engineering and Petrochemical, Laboratory of Applied Chemistry and the Environment, University of El Oued, El-Oued, Algeria,
[4]Institut des Sciences et des Techniques Appliquées, Laboratory of Silicates, Polymers and Nanocomposites (LSPN), Frères Mentouri University Constantine 1
Corresponding author: Kouadri Imane (imane.kouadri@gmail.com)

Abstract

Polluted water is still a major environmental problem around the world that needs new and long-lasting solutions. Chitosan is a natural polysaccharide that has a lot of potential for cleaning water because it is biodegradable, biocompatible, and very good at absorbing things. Chitosan is usually made from the shells of crustaceans, but fungus chitosan from mushrooms is a more environmentally friendly option that works just as well with fewer problems. The main focus of this work is on getting mushroom-derived chitosan out of the ground, characterizing it, and using it to clean up water. Chitosan was taken out of Agaricus Bisporus using improved chemistry methods. It was then analyzed using several techniques, and the level of deacetylation (DD) of the chitosan from mushrooms was measured. The chitosan that was made was tested to see how well it could remove organic pollution, especially methylene blue (MB) and methyl orange (MO) dyes. The results showed that MB broke down very well after being exposed to UV light, while MO broke down much less slowly under the same conditions. These results show that chitosan from mushrooms could be a sustainable and useful material for cleaning water, providing an alternative to commonly used chitosan sources.

Keywords: Mushroom, Fungal Chitosan, Extraction, Characterization, Adsorption, Sustainable Water.

Green Engineering of Biopolymer–Metal Oxide Nanocomposites for Solar Photodegradation of Organic Dyes

Imane Kouadri [1], Bachir Ben Seghir [2], Abdelkrim Rebiai [3], Abdelheq Layachi [4]

[1] Department of Process Engineering, Laboratory of Industrial Analysis and Materials Engineering (LAGIM), University May 8 1945, Guelma, Algeria
[2] Department of Process Engineering and Petrochemical, Laboratory of Renewable Energy Development unit in Arid Zones (UDERZA), University of El Oued, El Oued, Algeria
[3] Department of Process Engineering and Petrochemical, Laboratory of Applied Chemistry and the Environment, University of El Oued, El-Oued, Algeria,
[4]Institut des Sciences et des Techniques Appliquées, Laboratory of Silicates, Polymers and Nanocomposites (LSPN), Frères Mentouri University Constantine 1
Corresponding author: Kouadri Imane (imane.kouadri@gmail.com)

Abstract

This research presents an eco-friendly synthesis of ZnO–MgO–Chitosan and ZnO–Fe_2O_3–Chitosan nanocomposites using mint leaf extract and mushroom-derived chitosan as natural reducing and stabilizing agents. The process requires no additional catalysts, relying on the bioactive compounds of mint (alkaloids, glycosides, tannins, phenolics, flavonoids, and terpenoids). The nanocomposites were characterized using UV-Vis and other several analyses. Their photocatalytic efficiency was evaluated for the degradation of methylene blue (MB) and methyl orange (MO) under solar irradiation. The ZnO–MgO–Chitosan nanocomposite exhibited outstanding performance, achieving 98% MB removal within 330 minutes. These results highlight the potential of biopolymer-based hybrid nanomaterials as sustainable, low-cost, and efficient candidates for environmentally friendly wastewater remediation.

Keywords: Green synthesis, Photocatalysis, Chitosan, Nanocomposites, Wastewater treatment, Organic Dyes.

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Structural, electronic and Thermodynamic properties of $KBeCl_3$ halide perovskites using FP-LAPW method.

Imene Beldi [1], Nassima Chouit [2], Manouba Slimani [2], Hocine Meradji[2] and Sebti Ghemid[2].

[1] Laboratory LSC, Department of Physics, Badji Mokhtar University Annaba, Algeria.

[2] Laboratory LPR, Department of Physics, Badji Mokhtar University Annaba, Algeria.

Corresponding author: Beldi Imene
E-mail : beldi_imene@yahoo.fr

Abstract

This study presents a first-principles investigation of the perovskite compound $KBeCl_3$ using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method within the framework of Density Functional Theory (DFT). Structural optimization confirms the stability of the cubic perovskite phase. The calculated lattice parameters are in good agreement with theoretical expectations. Electronic band structure analysis reveals the semiconducting nature of $KBeCl_3$, with an indirect band gap. Thermodynamic properties such as the Debye temperature, specific heat, and thermal expansion coefficient are also evaluated. The material exhibits favorable stability at high temperatures. These findings suggest that $KBeCl_3$ could be a promising candidate for optoelectronic or thermoelectric applications. Overall, the study provides valuable insights into the fundamental properties of this halide perovskite.

Keywords: Debye model, Thermal properties, DFT, wien2k

Structural and Microstructural Proprties of Ferrochromium Milled Powders

Ahlam Khadraoui[1], Wassila Tebib[1], Naoual Houaidji [1], Afef Brahimi [1]

[1]Materials Physico-Chemistry Laboratory, Science and Technology Faculty, Chadli Bendjedid - El Tarf University,
P.B. 73, El Tarf 36000, Algeria.
E-mail:a.khadraoui@univ-eltarf.dz

Abstract:

This work focuses on the study of some physical properties of the ferrochromium (FeCr) powders obtained by high-energy mechanical milling in a Retsch PM400 planetary mill at different milling times (4h and 8h). The characterization of the milled powders was performed using X-ray diffraction in a Bruker D8 diffractometer. The main objective is to understand the influence of the milling time on the structural and microstructural properties of the product.

The structural study revealed the formation of a solid solution of substitution Fe (Cr) with a body-centered cubic structure. Therefore, the evolution of the milling time leads to progressive reduction of the cristallite size and to the increase in the crystalline parameters and microstrain.

Keywords: Nanomaterials; Fe-Cr alloys; Mechanical alloying; X-ray diffraction.

First-Principles Investigation of the Structural, Electronic, and Optical Properties of 2D Germanene Nanomaterial

Khouloud GHERBI[1], Hafid BELKHIR[1], Mohamed Tahar KADRI[1]

[1]Department of physics, Laboratory of studies of Surfaces and Interfaces of Solid Matter (LESIMS), University of Badji Mokhtar, Annaba, Algeria

Corresponding author: Khouloud GHERBI

khouloud.gherbi@univ-annaba.dz

Abstract

The structural, electronic, and optical properties of two-dimensional nanomaterials like germanene have been systematically investigated using first-principles calculations based on Density Functional Theory (DFT). The structural optimization confirms the buckled honeycomb geometry characteristic of germanene, resulting from mixed sp^2–sp^3 hybridization of Ge atoms. The electronic band structure exhibits a linear dispersion around the Fermi level (Dirac Cone) at the K-point with a finite band gap induced by spin–orbit coupling, confirming the semi-metallic nature of pristine germanene. The total and partial density of states (DOS) analyses reveal that the low-energy electronic states are primarily governed by Ge-p orbitals. The charge density distribution illustrates strong covalent bonding between neighbouring Ge atoms with partial sp^2–sp^3 hybridization. Furthermore, we explore the material's optical response by calculating the real and imaginary components of the dielectric function, absorption coefficient, and reflectivity of germanene, the results show pronounced anisotropy and strong absorption across the visible and ultraviolet regions, primarily driven by $\boldsymbol{\pi \rightarrow \pi^*}$ transitions. Key absorption peaks are identified and attributed to specific interband transitions, between π- and σ-bonding states in the VB and π^*- and σ^*-antibonding states in the CB. Germanene exhibits a high reflectivity (~35%) in the infrared-visible range (IR-VIS), which rapidly decreases beyond the plasma frequency (ω_p) at 4.8 eV, highlighting the material's potential for optoelectronic applications, such as photodetectors and transparent conductors. These theoretical insights into the fundamental electronic and optical characteristics of germanene provide a strong foundation for its future experimental realization and nanotechnology industries.

Keywords: 2D, germanene, buckled, DFT, electronic properties, optical properties.

Thermodynamic Assessment of Cellulosic Fiber Pyrolysis Using the Coats–Redfern Method

Lalaymia Imen*, Belaadi Ahmed[2]

[1]Department of Mechanical Engineering, Faculty of Technology, University 20 August 1955-Skikda, El-Hadaiek Skikda, Algeria;

[2]Laboratory LGMM, University 20 August 1955- Skikda, El-Hadaiek Skikda, Algeria

Email: * lalaymiaimen23@gmail.com

Abstract

This study employed thermogravimetric analysis (TGA) in combination with the Coats–Redfern method (CRM) to investigate the kinetic and thermodynamic aspects of the thermal degradation of fibers extracted from the flower stalk of Agave americana (FSAA). The thermal behavior of FSAA fibers was examined at different heating rates (5, 10, and 20 °C/min) to better understand their complex reaction mechanisms and estimate key kinetic parameters. The TGA results revealed a multi-step degradation process with strong correlation coefficients ($R^2 > 0.99$) across all heating rates. The calculated activation energies ranged from 83.6 to 210.1 kJ/mol, indicating that the decomposition kinetics were influenced by the heating rate. Thermodynamic parameters including changes in entropy (ΔS), Gibbs free energy (ΔG), and enthalpy (ΔH) provided insights into the spontaneity and energy transfer during degradation. The negative ΔS values suggested a decrease in molecular disorder as the reaction progressed. This research represents the first comprehensive investigation of the thermal behavior of FSAA fibers using CRM coupled with TGA. The results deepen the understanding of FSAA fiber decomposition mechanisms and highlight their potential for applications in biofuel production and sustainable composite materials.

Keywords: Pyrolysis, Cellulosic fiber, Coats–Redfern method, Thermodynamic analysis

Synthesis and Crystal Structure of Organic-Inorganic Materials Based on Amine Derivative

Laroum Rima[1,2], Gheribi Rima[3,4]

[1] Département Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Université Larbi Ben M'Hidi, Oum El Bouaghi 04000, Algérie

[2]Laboratoire de Synthèse des Molécules d'Intérêts Biologiques, Université des Frères Mentouri Constantine, 25000 Constantine, Algérie

[3]Unité de recherche de chimie de l'environnement et moléculaire structurale (CHEMS) Université des Frères Mentouri Constantine, 25000 Constantine, Algérie

[4]Département Sciences et Technologie, Faculté des Sciences et Sciences Appliquées, Université Larbi Ben M'Hidi, Oum El Bouaghi 04000, Algérie

Laroum Rima (laroum.rima@gmail.com)

Abstract

A key objective in crystal engineering is to create crystals with predictable structures and desirable properties for diverse applications, including electrical, agricultural, gas storage, and biological uses. Our research focuses on developing hybrid materials cantered on tin, combined with dicarboxylate acids (specifically oxalate) and organic amines. The properties of these materials are determined by their crystalline structure and the binding energies, particularly hydrogen bonding, which also helps establish connections between chemistry, biology, and biotechnology. The target compound was synthesized using a soft chemical approach. The compound consists of 2-aminopyridinium cations and a stannate (IV) dianion. In the anion, the tin (IV) center features an octahedral geometry, coordinated by two bidentate oxalate ligands and two chloride anions in a cis arrangement. The crystal packing is stabilized by N—H···O and C—H···O hydrogen bonds, creating an open framework.

Keywords: Hydrogen bond, Hybrid materials, Organic-inorganic materials, X ray.

Structural, morphological and optical properties of $CuInSe_2$ deposited on glass substrate by co-evaporation technique

Linda. SAAD-HAMIDECHE [1,*], Hayette. BENZEROUK [2], Fairouz. CHOUIT [2].

[1] Departement of Physics, Faculty of Ssciences Exactes, University of Frères Mentouri, Constantine 1, Constantine 25000, Algeria.

[2] Departement of technology, Faculty of Technology, 20 Aout 1955, University, P.O 26, Road El-Hadaik, Skikda, 21000, Algeria.

* Laboratory of LEREC, Departement of Physics, Faculty of Ssciences Exactes, University of Badji Mokhtar, Annaba, 2300, Algeria.

Corresponding author: saadhamideche.linda@umc.edu.dz

Abstract

$CuInSe_2$ thin layer were grown directly on glass substrate by co-evaporation technique. The analysis of X-ray (XRD) has revealed the existence of chalcopyrite phase depending on the direction (112) plane at time of milling 30 min. The analysis by scanning electron microscope (SEM) has observed that this material has fine microstructure. The optical gap of $CuInSe_2$ layer was fond around 1,02 eV by reflectance measurements.

Keywords: $CuInSe_2$, thin layer, chalcopyrite, X-ray, SEM, optical gap.

Cadmium Ion and Acetaminophen Removal from Aqueous Solution Using Chitosan Beads Prepared from Shrimp Shell Extracted Chitosan

M. Bendjaballah[a*], M. R. Makhlouf[a]

[a]Industrial Analysis and Materials Engineering Laboratory 8 May 1945 Guelma University B.P 401 Guelma 2400.

[b]National Polytechnic School of Constantine, Department of Process Engineering, Laboratory of Process Engineering for Sustainable Development and Health Products, BP 75, A, Nouvelle Ville RP, Constantine, Algeria.

[*] Corresponding author: bendjaballah.malek@univ-guelma.dz

Abstract

In this study, chitosan was derived from Parapenaeus longirostris shrimp shells sourced from a local market in Annaba, eastern Algeria. The extraction process entailed four chemical stages: demineralization, deproteinization, decolorization, and deacetylation. The degree of deacetylation was calculated to be 80.86 %. The extracted chitosan was physically altered to synthesize chitosan beads and characterized via FTIR and XRD analysis. These beads were employed to eliminate cadmium ions and acetaminophen (AAP) (paracetamol) from synthetic water. The batch adsorption process was optimized by analyzing the impact of contact time, pH, adsorbent dose, and temperature. The adsorption capacity of and Cd^{+2} AAP on chitosan beads was found to be 6.83 mg/g and 7.94 mg/g, respectively. The kinetic adsorption of Cd^{+2} and App conformed to the pseudo-first-order model, while the isotherm study indicated that the Langmuir Isotherm model well described the adsorption of cadmium and App. A thermodynamic analysis demonstrated that the adsorption of Cd^{+2} and AAP on chitosan beads is spontaneous and exothermic.

Keywords: Cadmium; Acetaminophen; Chitosan; Chitosan Beads; Biodsorption.

ACKNOWLEDGMENT

We would like to acknowledge the support provided by the Algerian Ministry of Higher Education for funding this research project. We are also grateful to the staff of the LAIGM laboratory for their technical assistance and to the participants who volunteered for this study.

Green formulation of Water-Based drilling Mud (WBM) with low cost: substitution of polymers by agricultural wastes Locust Bean Gum LBG

Malek BENDJABALLAH [a,*], Hacina SAIDI [b],

[a]Industrial Analysis and Materials Engineering Laboratory 8 May 1945 Guelma University P.O 401 Guelma 2400.
[b]Université Chadli Bendjedid El Tarf, Faculté Sciences de la nature et de la vie, 36000 El Tarf, Laboratoire des sciences de l'environnement et d'agroécologie, El Tarf.

Corresponding author: malekbendjabal@gmail.com

Abstract

Currently in the field of oil well drilling, research tends to use new technologies including alternative components for drilling fluids. Among the compounds that can be used in drilling fluids, carob nuts. The aspect of this project has been inserted into a section for the recovery of agricultural waste in order to minimize the degradation of the natural environment. This part of the work focused on the development of a biopolymer derived from carob nuts because of its techno-functional properties (stabilizer, thickener, binder and gelatinizer). In order to enhance the carob grains, preliminary treatments were carried out: Acid shelling (maceration), washing, soaking, drying and grinding operations. During this work, we wanted to check the conformity and study the performance of locust bean gum, which is a biodegradable biopolymer of plant origin derived from biomass, obtained locally, that we are substituting for other conventional products in the field of water-based Muds drilling fluids.

In particular we have studied the effect of carob gum as a filtrate reduction instead of polyanionic cellulose (PAC LV), and as a viscosifying instead of Xanthane gum which are imported biopolymers. These polymers often increase the cost price of a drilling operation.

Finally a water-based drilling mud formulated using environmentally friendly and low-cost locust bean gum has been developed by substituting total and partial biopolymer of Xanthan Gum (PAC LV) giving better rheological properties and flow control. Fluid loss requirements necessary for proper oil well drilling operation.

Keywords: Drilling, Drilling fluid, Biopolymers, Rheological.

First-Principles Investigation of The Structural, Electronic, and Thermodynamic Properties of The Perovskite $KBeBr_3$ via the FP-LAPW Method

Manouba Slimani [1], Nassima Chouit [1], Imene Beldi [1], Sebti Ghemid[1], and Hocine Meradji[1]

[1] Laboratory LPR, Department of Physics, Badji Mokhtar University Annaba, Algeria.

Corresponding author: Slimani Menouba

e-mail: menoubas@yahoo.fr

Abstract

in this work, we perform a first-principles study of the perovskite compound $KBeBr_3$ using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method within Density Functional Theory (DFT). The structural analysis confirms the mechanical stability and equilibrium geometry of the cubic phase. The optimized lattice parameters show consistency with the expected trends for halide perovskites. The electronic band structure reveals that $KBeBr_3$ is a wide-band-gap semiconductor, with an indirect band gap. Thermodynamic quantities such as bulk modulus, Debye temperature, and specific heat are computed to assess the material's thermal stability. The results suggest that $KBeBr_3$ maintains good structural and thermodynamic integrity under temperature variations. These findings highlight the potential of $KBeBr_3$ for applications in optoelectronics and energy-related technologies. This study contributes to the understanding of less-explored bromide-based perovskites

Keywords: FP-LAPW method, Thermodynamic properties, Halide perovskite, wien2k

Green Nanoparticle Synthesis for Vector Management: Sustainable Strategies Targeting Medically and Veterinarily Important Insects with a Focus on Diptera Culicidae

Mouna Cherairia[1], Samia Benrabah[2], Nedjoua Cheghib [3], Boumaza Awatif [1] & Larafa Amira[1,4]

[1] Department of Biology, University 8Mai 1945 Guelma, Guelma, Algeria
[2] Department of Geology, Geology Research Laboratory, Badji Mokhtar Annaba University, Annaba, Algeria
[3]Department of Material Sciences, Applied chemistry Laboratory, University 8Mai 1945 Guelma, Guelma, Algeria
[4] Department of Biology, Laboratory of Biology, Water and Environment, University 8Mai 1945 Guelma, Guelma, Algeria
Corresponding author: Mouna Cherairia (monachairi@yahoo.fr)

Abstract

Animals and humans are increasingly vulnerable to various diseases, particularly parasitic infections transmitted directly or through insect vectors. Mosquitoes (Diptera: Culicidae) are of major medical and veterinary significance, acting as vectors for a wide range of pathogens, including protozoa, viruses, bacteria, and nematodes. Diseases such as malaria (transmitted by Anopheles), filariasis, yellow fever, dengue fever, Japanese encephalitis in humans, as well as bovine malaria and brucellosis in animals, continue to pose serious health challenges. These risks are further amplified by climate change, which fosters the expansion and proliferation of mosquito populations. To address these challenges, several vector control strategies have been adopted, including chemical insecticides and plant-derived compounds. However, increased concerns regarding environmental toxicity and the rapid emergence of insecticide resistance have encouraged the exploration of innovative, ecofriendly alternatives. In this context, nanomaterial particularly green synthesized bionanoparticles, have emerged as a promising field**,** offering new avenues for the sustainable control of mosquito vectors such as Culex species.

Green synthesized nanoparticles exhibit potent larvicidal activity by inducing mortality and disrupting larval development at low, environmentally safe concentrations. As functional nanomaterials, they can be engineered to ensure controlled insecticide release by adhering to the larval cuticle or being ingested, enabling slow and targeted delivery of active molecules. This enhances larvicidal efficiency while minimizing ecological impact on aquatic environments.

The integration of nanomaterial-based, ecofriendly strategies represents a sustainable and effective approach to Culex mosquito larval control. These methods reduce the limitations associated with conventional chemical insecticides, protect aquatic ecosystems, and support long-term sustainability in vector management programs aimed at reducing mosquito-borne diseases affecting both humans and animals.

Keywords: Green nanotechnology, Bionanoparticles, Biosynthesis, Insecticide resistance Ecofriendly vector control.

Elaboration and Characterization of Nanocomposites Based on Polycarbonate and Linear Low-Density Polyethylene (PC/LLDPE/MMT)

Nadjat Chelghoum [1,3], Imen Meyouf [2] and Malea Guessoum [3].

1 Laboratoire de génie de l'environnement, Département de Génie des Procédés, Faculté de Technologie, Université badji mokhtar, Annaba, Algérie ;
[2]Laboratoire de Physico-Chimie des Hauts Polymères (LPCHP), Département de Génie des Procédés, Sétif1, centre Universitaire Abdelhfid boussouf Mila, Mila, Algérie ;
[3]Laboratoire de Physico- Chimie des Hauts Polymères (LPCHP), Département de Génie des Procédés, Faculté Technologie, Université Ferhat ABBAS Sétif1, Sétif, Algérie
Corresponding author: nadjat.chelghoum@univ-annaba.dz

Abstract

At the beginning of the 1990s, a new family of materials emerged, known as nanocomposites. They are characterized by the dispersion of aluminosilicate layers on the nanometer scale within polymer matrices. This results in improved mechanical and thermal properties of the polymer, even with low weight fractions of the dispersed filler.

The objective of this study is the elaboration and characterization of a polycarbonate/linear low-density polyethylene (PC/LLDPE) blend (70/30) and nanocomposites containing 1, 3, and 5% of organophilic montmorillonite (MMT), aiming to enhance thermal stability, mechanical properties, and viscoelastic behavior.

The PC/LLDPE/MMT nanocomposites were prepared using an internal mixer and characterized by Differential Scanning Calorimetry (DSC), torque rheometry, Melt Flow Index (MFI) measurement, and impact resistance (Izod) testing.

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Keywords: Blend, nanocomposites, polycarbonate, linear low-density polyethylene, montmorillonite.

Magnetic and structural properties of iron nanomaterials processing by mechanical alloying

Naouaem Boudinar[1,2], Nawel Nedjah1, Abdelmalik Djekoun2, and Bouguerra Bouzabata[2]

[1] Département de génie des Procédés et énergétique, Laboratoire de Technologies des Systèmes Energétiques LTSE, National Higher School of Technology and Engineering ENSTI, 23005 Annaba, Algeria ;
[2] Département de Physique, Laboratoire de Magnétisme et de Spectroscopie des Solides, Université Badji Mokhtar, Faculté des sciences, BP12 Sidi Amar, 23000 Annaba, Algeria.
Corresponding author: n.boudinar@ensti-annaba.dz

Abstract:

Magnetic iron nanomaterials were prepared facilely by mechanical alloying process. The solid-solution of Cu-50 wt% Fe and Ni-50 wt% Fe were prepared by ball milling of elemental powders up to 24 h. As-synthesized nanomaterials were characterized by means of SEM, XRD and VSM techniques. Results show as-prepared magnetic nanomaterials are sphere particles with aggregation state and magnetic α-Fe particles are enclosed by copper matrixes for Cu-50 wt% Fe and nickel matrixes for Ni-50 wt% Fe. It was found that the iron peaks in the XRD patterns vanish at the early stages of mechanical alloying process but the dissolution of Fe needs more milling time. Moreover, the crystallite size of the matrix decreases with increasing milling time and the crystallite size reaches a plateau with continued milling. The obvious magnetic hysteresis loops of the sample Cu-50 wt% Fe and Ni-50 wt% Fe indicate that these two samples have clear ferromagnetic characteristics.

Keywords: nanomaterials, mechanical alloying, magnetic properties, crystallite size refinement.

A DFT investigation on structural, electronic and thermodynamic properties of cubic perovskite SrLiF3

Nassima Chouit [1], Imene Beldi [1], Manouba Slimani [1], Hocine Meradji[1] and Sebti Ghemid[1]

[1]Laboratory LPR, Department of Physics, Badji Mokhtar University Annaba, Algeria.

Corresponding author: Chouit Nassima

e-mail: n_chouit@yahoo.fr

Abstract

In this work, we study the structural, electronic and thermodynamic properties of the cubic perovskite-type SrLiF3, using the full-potential linearized augmented plane wave method within density functional theory. We used the local density approximation LDA and the generalized gradient approximation GGA. The ground state properties such as lattice constants and bulk modulus are in good agreement with numerous experimental and theoretical data. The quasi-harmonic Debye model, using a set of total energy versus volume calculations obtained with FP-LAPW method is applied to study the thermal and vibration affects. Temperature effect on the lattice parameter, bulk modulus, thermal expansion coefficient, heat capacity and Debye temperature is calculated from the non-equilibrium Gibbs function.

Keywords: Debye model, FP-LAPW, Thermal properties, DFT

Biosynthesis of Zinc Oxide Nanoparticles Using (Zygophyllum album. L) Extract and Evaluation of Their Antibacterial Activity

mohammed said nedjimi[1], hayat zerrouki[1], mohamed lakhder belfar[1], Ben Moussa Wasam[1], Karboussa Ryan[1]

[1]VPRS Laboratory, Faculty of Mathematics & Matter Sciences, University of Kasdi Merbah, B.P. 511, 30000, Ouargla, Algeria
Corresponding author: mohammed said nedjimi (nedjimi2011@gmail.com)

Abstract

This research explores the eco-friendly synthesis of Zinc Oxide Nanoparticles (ZnO NPs) using an aqueous extract of the Zygophyllum album. L plant, commonly known as "Al-Aqqa," from southeastern Algeria. The extraction was efficiently performed using ultrasound-assisted methods, emphasizing the principles of green chemistry.

The synthesized ZnO NPs were characterized using several analytical techniques. UV-Vis spectroscopy confirmed nanoparticle formation with an absorption peak at 370 nm. FTIR analysis identified various functional groups from the plant extract involved in the reduction and stabilization of the nanoparticles. EDX and SEM analyses confirmed the presence of zinc and oxygen, the elemental composition of ZnO, and revealed a porous, high-surface-area morphology, albeit with some agglomeration.

A significant part of the study evaluated the antibacterial activity of the biosynthesized ZnO NPs against three pathogenic bacterial strains: Escherichia coli, Staphylococcus aureus, and Proteus. The results demonstrated a clear dose-dependent antibacterial effect. The highest concentration (10 mg/ml) showed the most substantial inhibition zones (17-18 mm), outperforming or matching the standard antibiotic (Gentamicin) in some cases against E. coli and Proteus. In conclusion, this research successfully established a simple, cost-effective, and environmentally friendly method for producing ZnO NPs using a local medicinal plant. The obtained nanoparticles exhibited promising antibacterial properties, highlighting their potential for applications in biomedical fields as antimicrobial agents, as well as in food preservation, water treatment, and cosmetics. This work represents a significant step towards sustainable nanomaterial production and encourages further research and development in this promising area..

Keywords: ZnO Nanoparticles, Zygophyllum album. L (Al-Aqqa), Ultrasound-Assisted Extraction, ntibacterial Activity, Green Synthesis

Substitutional doping of 3d transition metals in $NiCl_3$ monolayer: A systematic study

Norelhouda Salah[1], Hakima Yahi[2]

[1] Materials Physics Laboratory (L2PM), University May 8, 1945 Guelma, BP 401 Guelma 24000, Algeria

[2] Materials Physics Laboratory (L2PM), University May 8, 1945 Guelma, BP 401 Guelma 24000, Algeria

Corresponding author: Norelhouda Salah (norelhudasalah@gmail.com)

Abstract

Owing to their exceptional properties and potential for advanced applications in spintronic devices and data storage, two-dimensional van der Waals materials have garnered significant research interest. In this work, we perform first-principles calculations within the GGA + Ueff approach to comprehensively explore the structural and electronic characteristics of pristine and 3d transition metal (TM = V and Cr) doped $NiCl_3$ monolayers. In particular, V-doped monolayer exhibit half-semiconducting (HSC) characteristics, while Cr-doped system display features of bipolar ferromagnetic semiconductors (BFMS). Furthermore, by introducing spin–orbit coupling (SOC) into the simulated monolayers, we demonstrated its influence on the band gap widths. We also observed robust ferromagnetic stability across all doped systems, along with a significant enhancement of the total magnetic moment, reaching up to 15 μB in the Cr-doped monolayer. These compelling insights into the electronic and magnetic properties of pristine and transition metal-doped $NiCl_3$ monolayers offer promising opportunities for the development and optimization of next-generation electronic and spintronic devices.

Keywords: 2D materials, ferromagnetism, TM doping, semiconductivity, spintronics

Hydrogen Storage in two-dimensional (2d) Materials, DFT calculation

Ouarda Benamara[1], Karima Akroud[1], Kamel Zanat[1]

[1]Depatement of Matter Science, Guelma Physics Laboratory (GPL), University 8 Mai 1945, BP 401, Guelma, Algeria.
Benamara Ouarda ; benamara_war@yahoo.fr

Abstract

Hydrogen storage is a major challenge in developing clean energy technologies, leading to growing interest in two-dimensional (2D) materials due to their unique structural and electronic properties. This work presents a theoretical study of hydrogen molecule adsorption on molybdenum diselenide (MoSe2), a material from the transition metal dichalcogenide (TMD) family. We used density functional theory (DFT) as implemented in the open-source Quantum ESPRESSO code. Calculations were performed using a norm-conserving pseudopotential in two steps : first, studying the pure MoSe2 surface, and then examining the structure modified by atomic decoration through substituting a Selenium atom with a copper (Cu) atom. This approach aims to enhance the material's adsorption capacity by generating new, more reactive active sites. The results show that metallic decoration significantly improves the adsorption behavior, reaching conditions close to the ideal range for reversible storage. This highlights the potential of modified MoSe2 as a promising candidate for solid-state hydrogen storage applications.

Key words: two-dimensional (2D), Hydrogen storage, DFT, MoSe2. Clean energy.

Élaboration et caractérisation des nanoparticules d'oxyde de zinc (ZnO) à usage antimicrobien

Radia MEKAHLIA [a] *, Abdelali MERAH [b], Samia BOULEDROUA[b], Leila MEKAHLIA[b]

[a] Laboratoire central, Etablissement Public Hospitalier El Hadjar, Annaba

[b] Laboratoire de Chimie Minérale, Département de Pharmacie, Faculté de Médecine, Annaba

E-mail : radiamekahlia@gmail.com

Résumé :

Les nanoparticules d'oxyde de zinc (ZnO) suscitent un intérêt croissant en raison de leurs propriétés physico-chimiques remarquables et de leurs multiples applications biomédicales et industrielles. Elles sont notamment utilisées comme agents antimicrobiens, supports de vectorisation de principes actifs, filtres UV dans les écrans solaires ou encore additifs fonctionnels dans divers produits pharmaceutiques et cosmétiques.

L'objectif de ce travail est l'élaboration de nanoparticules de ZnO pur et leur caractérisation par des techniques structurales, morphologiques et spectroscopiques. Les nanoparticules ont été synthétisées par la méthode de précipitation, puis caractérisées par spectroscopie UV- Visible, spectroscopie infrarouge à transformée de Fourier (FT-IR), microscopie électronique à balayage (MEB) couplée à la spectroscopie dispersive d'énergie (EDS), et diffraction des rayons X (DRX).

L'analyse optique (UV-Vis) a révélé un maximum d'absorbance à 379,88 nm, confirmant la formation du ZnO. Les spectres FT-IR ont mis en évidence les bandes caractéristiques des liaisons métal-oxygène (Zn–O). L'observation MEB a montré des particules sphéroïdales de taille nanométrique, tandis que l'analyse EDS a confirmé une pureté chimique élevée. Les diagrammes de DRX ont révélé une structure cristalline hexagonale de type wurtzite, avec une taille moyenne de cristallites de 54,5 nm.

Ces résultats démontrent que la méthode de précipitation permet d'obtenir des nanoparticules de ZnO de bonne pureté, à faible coût, et présentant un fort potentiel pour des applications antimicrobiennes.

Mots-clés : nanoparticules, oxyde de zinc, précipitation, caractérisation, propriétés antimicrobiennes.

Smooth Surface Morphology and Wide Band Gap of Pure Sol-Gel ZnO

Samah Boudour[1], Idris Bouchama[2], Salim Ali Saoucha[2]

[1] Research Center in Industrial Technologies CRTI, P.O. Box 64, Cheraga, 16014, Algiers, Algeria
Department of Electronic, Faculty of Technology, University of Mohamed Boudiaf, M'sila, 28000, Algeria
Corresponding author: Samah Boudour (s.boudour@crti.dz)

Abstract

Pure ZnO sample was prepared using a sol gel spin-coating technique on glass substrate, exhibiting a crystalline hexagonal zincite structure. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) revealed a micro-granular morphology for ZnO surface, where the substrate was completely covered by spherical-like grains. Optically, ZnO displayed a wide band gap energy of 3.26 eV. Key structural and surface properties include a 39 nm crystallite size, an arithmetic mean height (S_a) 0.035+0.002 µm indicating a smoother, more uniform surface, and a -0.061+0.003 (S_{sk}) reflecting a minor valley-dominated surface topography. This combination of high crystallinity and surface uniformity makes it highly suitable as an Electron Transport Layer (ETL) or a Transparent Conducting Oxide (TCO) in photovoltaic devices (like solar cells) and for use in UV photodetectors.

Keywords: ZnO, Spin Coating, crystallinity, topography,

Tuning Electronic and Mechanical Properties of a 2D Transition Metal Carbide via Density Functional Theory

Hakima Yahi and Hossayn Chibani

Department of Matter Sciences, Materials Physics Laboratory (L2PM), University May 8-1945, Guelma, Algeria

yahi.hakima@univ-guelma.dz

Abstract

Over the past few decades, two-dimensional (2D) materials have attracted significant attention due to their exceptional physical and chemical properties, which make them highly promising for a wide range of applications in nanotechnology, electronics, and energy storage.
In this study, we investigate the structural, electronic, and mechanical properties of novel 2D transition metal carbide, employing spin-polarized density functional theory (DFT) calculations. This material belongs to the M_4C_3-type MXene family, which is known for its versatility and tunable characteristics. To ensure accuracy and reliability in our predictions, we employed several exchanges–correlation functionals, including PBE, PBE+U, SCAN, and the hybrid functional HSE06. Our findings indicate that the studied MXene is mechanically robust and elastically isotropic, with a mechanical strength that is comparable to that of graphene, one of the most well-known 2D materials. Furthermore, the system demonstrates thermodynamic and dynamic stability, and exhibits metallic behavior across all computational approximations used. Notably, it also displays intrinsic magnetism in its ground state, a feature often associated with group IV-based MXenes. These results offer valuable insights into the fundamental properties of this MXene and underscore its potential for future use in nanoelectronic, spintronic, and other advanced nanotechnological devices. Our theoretical analysis lays a foundation for experimental exploration and design of novel MXene-based compounds with tailored properties.

Keywords: Structural Properties, Mechanical Properties, first principal calculations, Monolayer.

Theoretical Investigation of the Structural, Electronic, and Magnetic Properties of a Two-Dimensional Transition Metal Trihalide

Hakima Yahi and Chaouki Ouettar

Department of Matter Sciences, Materials Physics Laboratory (L2PM), University May 8-1945, Guelma, Algeria

yahi.hakima@univ-guelma.dz

Abstract

In this work, we present a comprehensive theoretical investigation of the structural, electronic, and magnetic properties of a two-dimensional molybdenum triiodide (MoI_3) monolayer. The calculations were performed using the projector augmented wave (PAW) method within the framework of density functional theory (DFT), as implemented in the Vienna Ab initio Simulation Package (VASP). Exchange–correlation effects were treated using the generalized gradient approximation (GGA), ensuring a reliable description of the system's ground-state properties. To evaluate the thermodynamic stability of the MoI_3 monolayer, formation energy calculations were carried out under varying chemical potential conditions. The results reveal that the monolayer is thermodynamically stable, with more favorable formation energy under iodine-rich (I-rich) conditions compared to molybdenum-rich (Mo-rich) conditions. This indicates that synthesis under I-rich environments could be more energetically favorable and experimentally viable. Furthermore, detailed analysis of the electronic band structure and projected density of states (PDOS) reveals that the monolayer exhibits a distinct magnetic character. The results confirm that the material behaves as a bipolar ferromagnetic semiconductor (BFMS), a rare and promising class of materials characterized by spin- polarized charge carriers in both the conduction and valence bands. This dual spin polarization is particularly attractive for next-generation spintronic applications, where control over both charge and spin degrees of freedom is essential. The combination of thermodynamic stability, semiconducting behavior, and intrinsic ferromagnetism makes this 2D system a strong candidate for integration into future nanoelectronic and spintronic devices.
These findings not only contribute to the fundamental understanding of transition metal trihalide monolayers but also open new avenues for the design of functional magnetic nanomaterials with tailored properties.

Keywords: Electronic properties, Magnetic properties, First principle calculations, Ferromagnetic semiconductor, Monolayer.

Diluted Semiconductor (BaK)F (ZnMn)As with Decoupled Charge and Spin Doping, First Principal Study

Yasmina Azouz[1], Kamel Zanat[1]

[1] Laboratoire de Physique de Guelma LPG, Université 8 Mai 1945 Guelma, Algérie

Corresponding author: Yasmina Azouz (azzyas2012@gmail.com)

Abstract

In this work, we have performed an ab-initio study for BaKFZnMnAs compounds where the co-doped K and Mn substitutional ordering are for hole and spin doping, respectively, using the most important exchange-correlation functionals on the parent compounds of the two limiting cases, of the magnetic compound BaFMnAs and the semiconductor BaFZnAs. We have evaluated the dependence of the exchange coupling parameter J0 on Mn pair distance dMn−Mn for spin concentrations of x=6%, 11%, and 25%.

Without hole doping, the interaction has an exponential damping with increasing dMn−Mn distance. Moreover, the interaction almost halved when going from 1N N to 2N N, maintaining its nature. This short and localized interaction characterizes the AF superexchange interaction or spin glass order. However, beyond the second neighbor the interaction is negligible.

Keywords: DMS, Ferromagnetic, Spin doping, Exchange-correlation

Low-Temperature Solvent-Free synthesis Route of Blue and Green Luminescent Phases of Tris(8-hydroxyquinoline) aluminum (AlQ3)

Karima Zerrouki [1], Rafika Bouchene [2,3] and Pascal Retailleau[4]

[1]Laboratoire de Chimie Appliquée et Technologie des Matériaux LCATM, Université d'Oum El Bouaghi, Oum El Bouaghi, 04000, Algeria,
[2] Département Sciences de la Matière, Faculté des Sciences Exactes et Sciences de la Nature et de la Vie, Universite d'Oum El Bouaghi, Oum El Bouaghi, 04000, Algeria
[3]Laboratoire des Sciences Analytiques, Matériaux et Environnement, Université d'Oum El Bouaghi, Oum El Bouaghi, 04000, Algeria,
[4]Institut de Chimie des Substances Naturelles, CNRS UPR 2301, Universit´e Paris-Saclay, 1 avenue de la Terrasse, Gif-sur-Yvette 91198, France.
Karima Zerrouki: E-mail: karima.zerrouki@univ-oeb.dz

Abstract

Even after more than 20 years of intensive research and development, tris(8-hydroxyquinolinato) aluminum (III) (widely abbreviated AlQ3) remains one of the most widely used materials for organic light-emitting diodes (OLEDs). AlQ3 is an octahedrally coordinated chelate complex wherein aluminium is bonded in a bidentate manner to the conjugate base of three 8-hydroxyquinoline (8-HQ) ligands.

According to the orientations of the ligands, the AlQ3 complex can occur in two isomeric forms; facial (fac) and meridional (mer). Depending on the type of isomers, the light emission of the complex changes from green (mer) to blue (fac). As reported in the literature, it has been established that the synthetic approaches used to prepare mer-AlQ3 are not suitable for the fabrication of the facial isomer. The fac-AlQ3 can only be obtained by solid phase conversion of the meridional isomer at very high temperatures.

On the other hand, with the increasing use of chemicals, scientists are increasingly aware of the environmental impact of their research activities and, therefore, the need to develop new environmentally friendly methodologies. Thus, by eliminating harmful and flammable organic solvents, solid-state synthesis methods have emerged as a green alternative.

In the context of soft reaction conditions and the concept of green chemistry, this investigation focused on the development of an easy-to-handle, efficient and environmentally friendly approach for the preparation of AlQ3 in the solid state under solvent-free conditions and at low temperature. To shift the equilibrium towards the reaction products, sodium carbonate is used as a solid support. Sodium carbonate is a very stable inorganic compound with alkalinizing properties that can deprotonate the organic ligand to promote the coordination interaction. The developed synthetic approach allowed the preparation of the mer and fac isomers under soft conditions.

Keywords: Green chemistry, Solide state reaction, tris(8-hydroxyquinolinato) aluminum (III), Sodium carbonate, Organic light-emitting diode (OLED).

Electrochemical Synthesis and Characterization of MnO_2/Carbon Cathode Materials

Zineb Nabti[1], Reda Bekhakhecha[2], Tarik Bordjiba[1], Manal Azouz[4], Nesrine Mezdoude[4].

[1]Laboratory of Electrical Engineering of Guelma (LGEG), Department of Process Engineering, Université 8 Mai 1945, Guelma 24000, Algeria.
[2]Laboratory of of Automation and Computer Science of Guelma (LAIG), Department of Electrical Engineeing and Automatic, Université 8 Mai 1945, Guelma 24000, Algeria
[3]Department of Process Engineering, Université 8 Mai 1945, Guelma 24000, Algeria.
Corresponding author: Zineb Nabti (midonabti@gmail.com)

Abstract

In this work, we present the electrochemical synthesis of manganese dioxide (MnO_2) deposited on a carbon substrate from an acidic bath. The electrodeposition potential was selected based on the manganese potential–pH diagram, allowing us to identify the thermodynamically favorable region for MnO_2 formation while avoiding competing reactions. The deposition was carried out at an applied potential of 1 V vs Ag/AgCl for 1 minute, and the performance was compared with that of an unmodified carbon substrate. The chronoamperometric response was used to analyze the initial nucleation and growth mechanism of MnO_2, as well as the stability of the deposition process. Morphological characterization was performed using optical microscopy, revealing the evolution of the surface before and after modification, and FTIR spectroscopy, confirming the presence of the characteristic Mn–O bands of the deposited MnO_2.

Electrochemical studies, conducted using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), showed a significant enhancement in the electrochemical activity of the modified electrode compared to bare carbon. The MnO_2-modified electrodes exhibited a more pronounced redox response, improved pseudocapacitive behavior, and a reduction in charge-transfer resistance, highlighting the relevance of MnO_2 for applications in Zn–ion battery systems.

Keywords: Electrochemical synthesis, Cathode materials, Carbon substrate, MnO_2 composites, Structural characterization, Electrochemical performance.

Theoretical Study of The Interaction Between the Protein Fibronectin and The Herbicide Terbutryn by Molecular Docking

Arab Houda [1], Masmoudi Rida [1], Khettaf Sami [1], Bouchekioua Saad [2], Dibi Ammar [1].

1Laboratory of Chemistry and Environmental Chemistry (LCCE), Department of Chemistry, Faculty of Material Sciences, University of Batna-1, Batna, Algeria.

2 Pharmaceutical Sciences Research Center (CRSP), Constantine, Algeria.

Corresponding author: Arab Houda (houda.arab@univ-batna.dz)

Abstract

It is important to highlight the significance of interactions between herbicides and biological applications. These herbicides, such as terbutryn, are widely used in agriculture, particularly in sugar cane, maize and rice crops, due to their effectiveness in eliminating weeds by inhibiting photosynthesis. However, chronic exposure to these herbicides represents a potential risk to human health. Recent studies have shown that triazines can interfere with cellular proteins. Such as Fibronectin 1 (FN1), involved in neuronal cell adhesion and synaptic stability, disruption of this protein is considered one of the main mechanisms in the development of Alzheimer's disease. So, despite their agricultural importance, the intensive use of terbutryn raises concerns about their neurotoxic effects and their potential role in increasing the risk of Alzheimer's disease.

Consequently, a simulation study has been proposed to investigate the interactions between terbutryn and the protein Fibronectin 1 (FN1). The use of molecular docking technique. The docking calculation was performed by AutoDock vina, 3D dimensional crystal structure of fibronectin 1 FN1 (PDB: 1FNF)). Was obtained from the protein database http://www.rcsb.org./pdb. The calculation of terbutryn were performed on using density functional theory (DFT) with the hybrid functional B3LYP at base 6-311++G (d, p) in isolated phase, using the Gaussian 16 package.

Keywords: DFT, Fibronectin 1 (FN1), Molecular docking, PDB, Terbutryn

ETUDE DE LA CATALYSE DANS LA REACTION DE HANTZSCH

Mennana Imene[1], Nemouchi Sara[1], Gherboudj Wissem[1]

[1]Departement de Chimie, Laboratoire SYMBIO, Université des frères Mentouri Constantine1, Constantine, Algérie

Mennana Imene (imene.mennana1@gmail.com)

Résumé :

Au vu de ce qui fait l'actualité des publications à travers la synthèse de nouveaux produits qui procréent et enrichissent les bibliothèques des familles de produits, la rénovation des voies synthétiques des produits cibles comme : Ampicilline, Atropine …etc. et l'élaboration de nouvelles voies plus respectueuses de l'environnement, nous percevons l'effervescence engendrée par le potentiel distinctif de la famille des réactions à composants multiples par rapport aux réactions classiques à deux composants ; de là est née notre évidence quant à cette famille de réactions, pour en faire un challenge.

une étude critique via les mécanismes proposés en milieu acide et en milieu basique pour en faire ressortir la nouvelle idée de la Co-catalyse acido-basique et d'en déterminer le couple FeCl3/DMAP, dont l'étude de détermination des conditions optimales a donné naissance à une nouvelle alternative de la catalyse dans la réaction de HANTSZCH.

Keywords: RMC; HANTSZCH.

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Faculty of Mathematics, Computer Science and Materials Science

Laboratory of Applied Chemistry (LCA)

BP. 401 University 8 May 1945 Guelma
24000 Algeria

Phone: +213.37116471
E-mail: 4.snca.2025@gmail.com