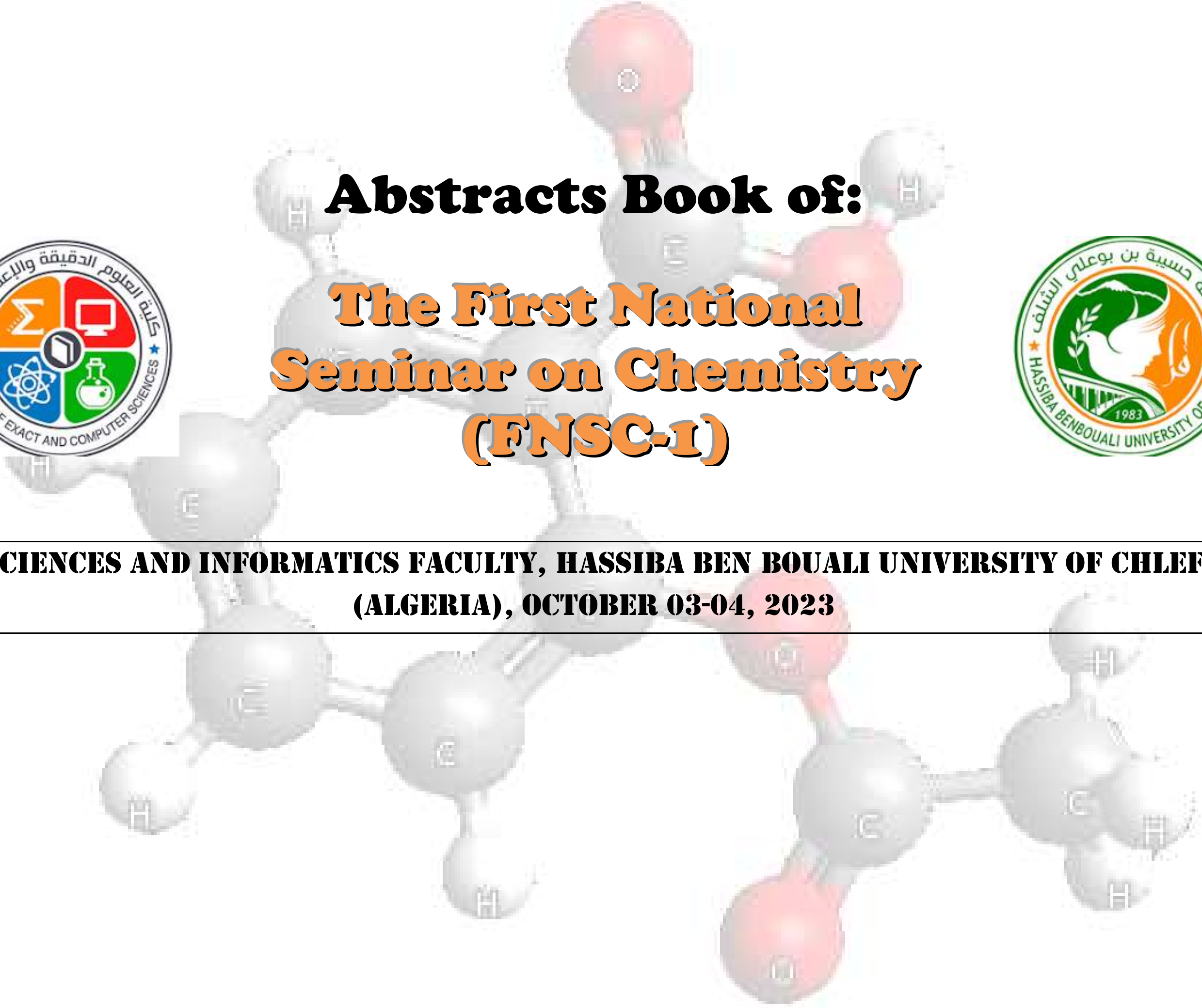
Revue Nature et Technologie
Academic Journal Edited By Hassiba BENBOUALI University
of Chlef (Algeria) under ISSN : 1112-9778
https://journals.univ-chlef.dz/index.php/natec/



Abstracts Book of:

The First National Seminar on Chemistry (FNSC-1)

SCIENCES AND INFORMATICS FACULTY, HASSIBA BEN BOUALI UNIVERSITY OF CHLEF
(ALGERIA), OCTOBER 03-04, 2023

Preface

Chemistry is an experimental science in the service of humanity. It is at the interface of several disciplines (Biology, Parachemistry, Health, Materials, Pharmacy, Environment, Electronics, Agronomy, etc.).

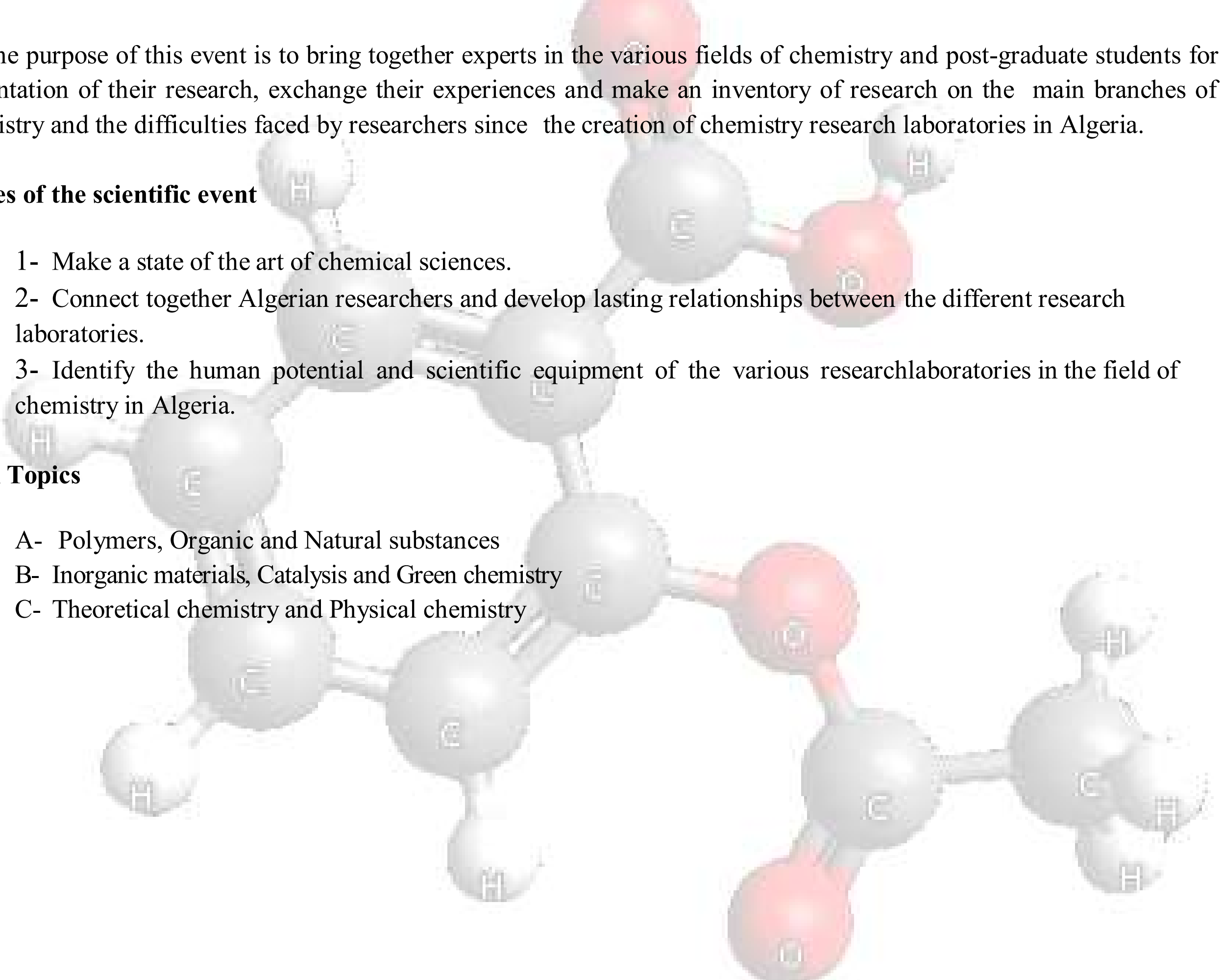
The purpose of this event is to bring together experts in the various fields of chemistry and post-graduate students for the presentation of their research, exchange their experiences and make an inventory of research on the main branches of the chemistry and the difficulties faced by researchers since the creation of chemistry research laboratories in Algeria.

Scopes of the scientific event

1- Make a state of the art of chemical sciences.
2- Connect together Algerian researchers and develop lasting relationships between the different research laboratories.
3- Identify the human potential and scientific equipment of the various researchlaboratories in the field of chemistry in Algeria.

Main Topics

A- Polymers, Organic and Natural substances
B- Inorganic materials, Catalysis and Green chemistry
C- Theoretical chemistry and Physical chemistry



Website: **https://www.univ-chlef.dz/FNSC1**
fnsc.chlef@gmail.com

Honorary Committee

Pr. ACHOUR Djilali.,	Rector of University Hassiba Ben Bouali Chlef
Pr. TAHAR ABBES Mounir	Dean of Exact Sciences and Informatics Faculty

Scientific Committee members

Chairman: Dr. HEDIDI Madani

.

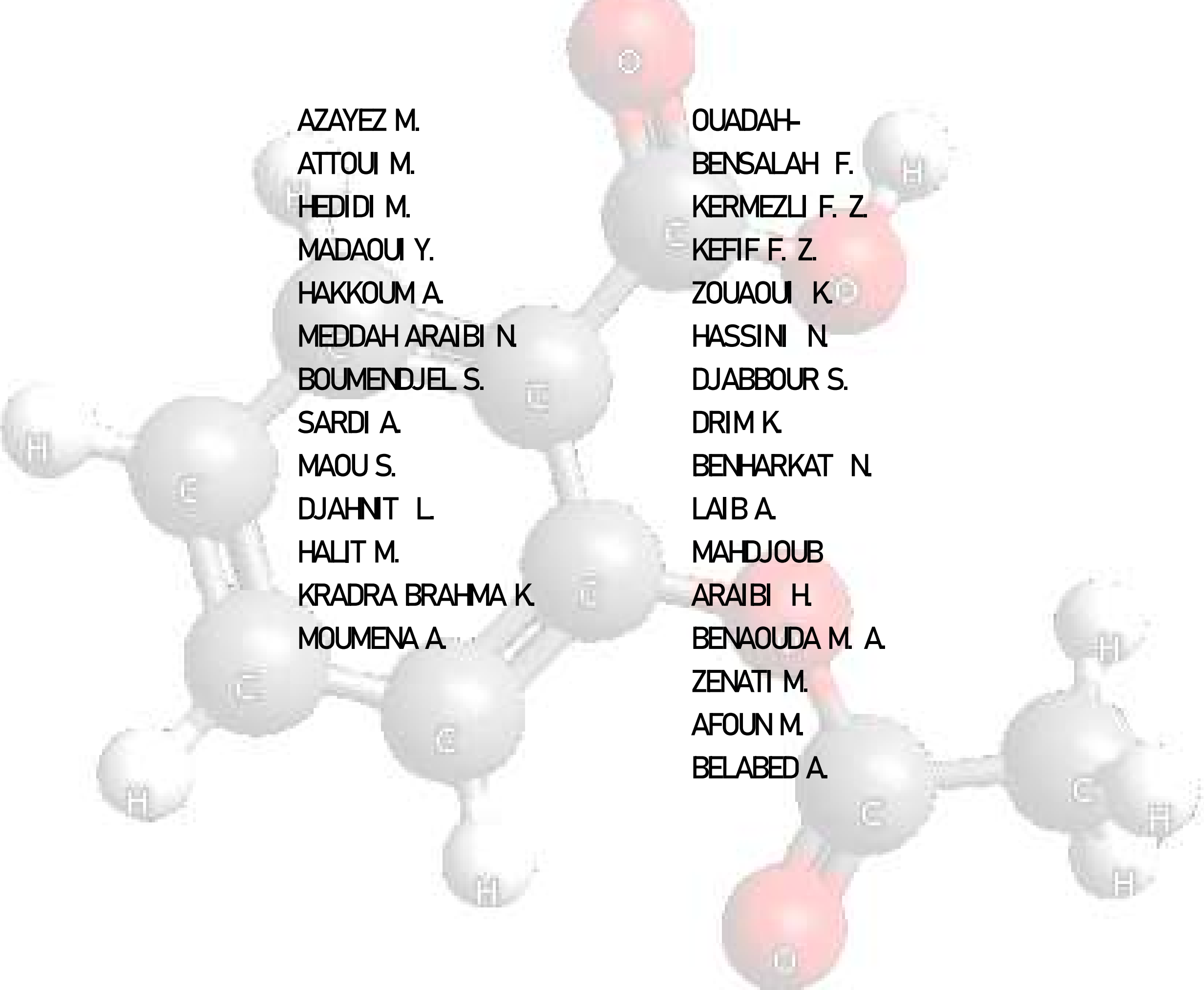
Pr. AMARA M., U. STHB
Pr. BACHIR R., U. Tlemcen
Pr. BENACHOUR D., U. Setif
Pr. BOUHADDA Y., U. Mascara
Pr. BOUKOUSSA B., USTO
Pr. BOUNACEUR B., U. Oran1
Pr. CHOUAIH A., U. Mostaganem
Pr. DRISSI M., U. Tiaret
Pr. EL MILOUDI K., U. Chlef
Pr. FERGOUG T., U. Mascara
Pr. HACHAMA K., U. Khemis Miliana
Pr. HAMACHA R., U. Oran1
Pr. HENINI G., U. Chlef
Pr. KHADRAOUI A., U. Khemis Miliana
Pr. LAIDANI Y., U. Chlef
Pr. MONGIN F., U. Rennes (France)
Pr. SAADI A., U. STHB
Pr. SAIDI S., U. Oran1
Pr. SALHI N., U. Blida
Pr. ZANOUN A., ENP Oran
Dr. AMEUR MESSAOUD M. Y., U. Chlef
Dr. BAILICHE Z., U. Ain Temouchent
Dr. BENDJELLOUL M., U. Relizane
Dr. BOUKABCHA N., U. Chlef
Dr. EL HORRI A. M., U. Chlef
Dr. ERB W., U. Rennes (France)
Dr. MEGROUS Y., U. Chlef
Dr. METLEF S., U. Chlef
Dr. MOKHTAR A., U. Relizane
Dr. MOUMENE T., U. Tiaret
Dr. SADOU M., U. Chlef
Dr. TAHRAOUI-DOUMA N., U. Chlef
Dr. ZIDANE A., U. Chlef
Dr. ZOUAOUI-RABAH M., ENPO

President of the Seminar

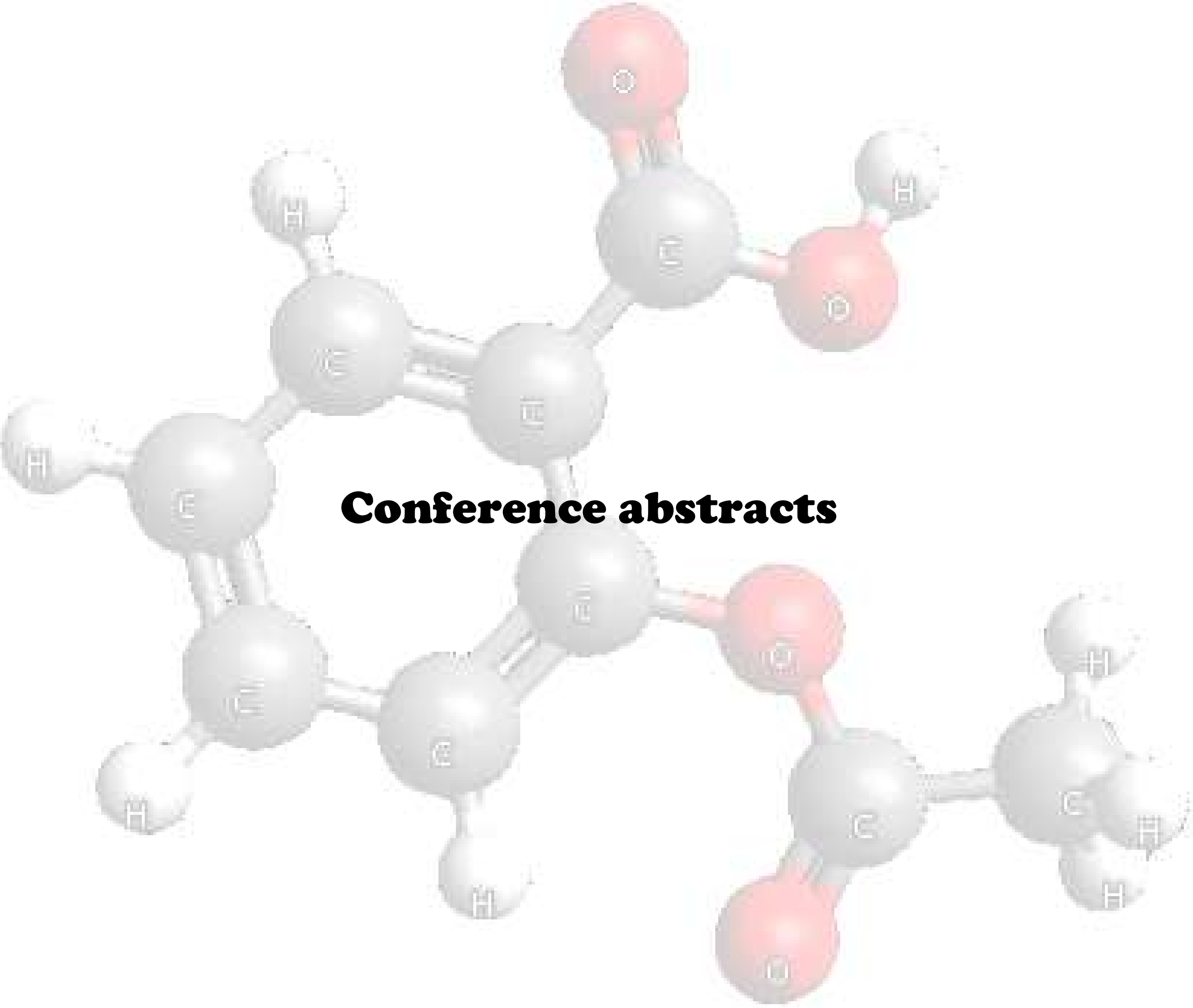
Dr. BENNABI S.

Organizing Committee members

Chairman: Dr. SADOU Mohamed



- AZAYEZ M.
- ATTOUI M.
- HEDIDI M.
- MADAOUI Y.
- HAKKOUM A.
- MEDDAH ARAIBI N.
- BOUMENDJEL S.
- SARDI A.
- MAOU S.
- DJAHNIT L.
- HALIT M.
- KRADRA BRAHMA K.
- MOUMENA A.
- OUADAH-BENSALAH F.
- KERMEZLI F. Z.
- KEFIF F. Z.
- ZOUAOUI K.
- HASSINI N.
- DJABBOUR S.
- DRIM K.
- BENHARKAT N.
- LAIB A.
- MAHDJOUB ARAIBI H.
- BENAOUDA M. A.
- ZENATI M.
- AFOUN M.
- BELABED A.



Conference abstracts

L'importance des éléments chimiques terres rares dans le développementtechnologiques

Pr. Mourad AMARA

Laboratoire d'hydrométallurgie, Faculté de Chimie, USTHB
mourad.amara@usthb.edu.dz

Résumé

Ces dernières années un grand nombre d'applications miniaturisées de haute technologies ne sont plus envisageables sans les terres rares, que ce soit dans les produits de notre vie quotidienne comme les Smartphones, et les téléviseurs à écran plat, ou dans le secteur des technologies vertes comme les aimants permanents superpuissants des éoliennes, les batteries des voitures électriques et hybrides, ou encore dans l'imagerie médicale, ou dans le secteur de l'armement pour le guidage des missiles.

Les terres rares sont une famille d'éléments chimiques constituée par les 15 lanthanides auxquels sont ajoutés l'yttrium et le scandium. Ces éléments possèdent des propriétés physico-chimiques très intéressantes et spécifiques et sont caractérisées par des similitudes notamment dans leur valence et leur taille. L'extraction de ces métaux se fait généralement grâce à l'exploitation des minerais primaires contenant la monazite, la bastnaésite ou la xénotime, mais peuvent également se trouver comme ressources secondaires contenus dans des minerais classiques de fer, de phosphate ou de bauxite par exemple.

Les techniques d'enrichissement et de séparation font appel à la lixiviation acide suivie par l'extraction par solvant ou la séparation par échange d'ions sur résines ou encore la filtration membranaire. Les techniques classiques sont à la fois couteuses et polluantes, mais les avancéesliées aux traitements et à la valorisation des rejets miniers rendent les opérations très attractives. Très souvent, les éléments majoritaires sont ceux appartenant au groupe des terres rares légèrestels que le lanthane, le cérium, le néodyme et le praséodyme. Ces deux derniers figurent cesdernières années sur la liste des métaux critiques où l'offre reste de loin inférieure à la demande.Le néodyme est utilisé dans la fabrication des aimants permanents les plus puissants de typeNdFeB.

Les travaux de recherches sont souvent orientés vers le choix des paramètres optimaux de séparation entre les différents éléments de cette famille exceptionnelle.

POLYMERES, ORGANIQUE ET SUBSTANCES NATURELLES

Dr. Meriem BENDJELLOUL

Université de Relizane
Corresponding Author: marybendjelloul@gmail.com

Résumé

Les polymères organiques appartiennent à une science qui a pris son essor dans les années 40. L'univers de la chimie des polymères s'est développé à un niveau tel qu'il ouvre désormais d'immenses possibilités à la créativité des chimistes. IL est possible maintenant de fabriquer de nouvelles substances, polymères, qui ont caractérisé par leur masse moléculaire et leur structure. La famille des polymères organiques est très vaste et subdivisée en deux grands groupes : les polymères naturels et les polymères synthétisés à base des monomères.

Durant ces dernières décennies les chercheurs aboutirent à la création de nouveaux polymères hyperbranchés les dendrimères. Selon Tomalia et Fréchet [10], les architectures macromoléculaires peuvent être divisées en quatre grandes familles : les polymères linéaires, ramifiés, réticulés et plus récemment les polymères dendritiques.

Dans un contexte de développement durable, les recherches sont orientées actuellement vers le développement de biotechnologies qui est consacré à l'utilisation des polymères naturels.

Parmi les polymères naturels on peut citer les déchets lignocellulosiques ou les polysaccharides (amidon, cellulose, chitine …), les protéines (caséine, gluten…). Ces polymères connaissent depuis quelques années un réel essor du fait de leurs origines naturelles et surtout de leur caractère biodégradable.

Récemment, plusieurs des études ont montré l'efficacité des polymères naturels et les polymères dendritiques pour le traitement de l'eau en raison de leur capacité d'élimination exceptionnelle, plus de surface et un grand nombre de sites actifs pour l'interaction avec les polluants.

TUNABLE HETEROCYCLIC MATERIALS FOR ADVANCED APPLICATIONS

Pr. Salima SAIDI-BESBES

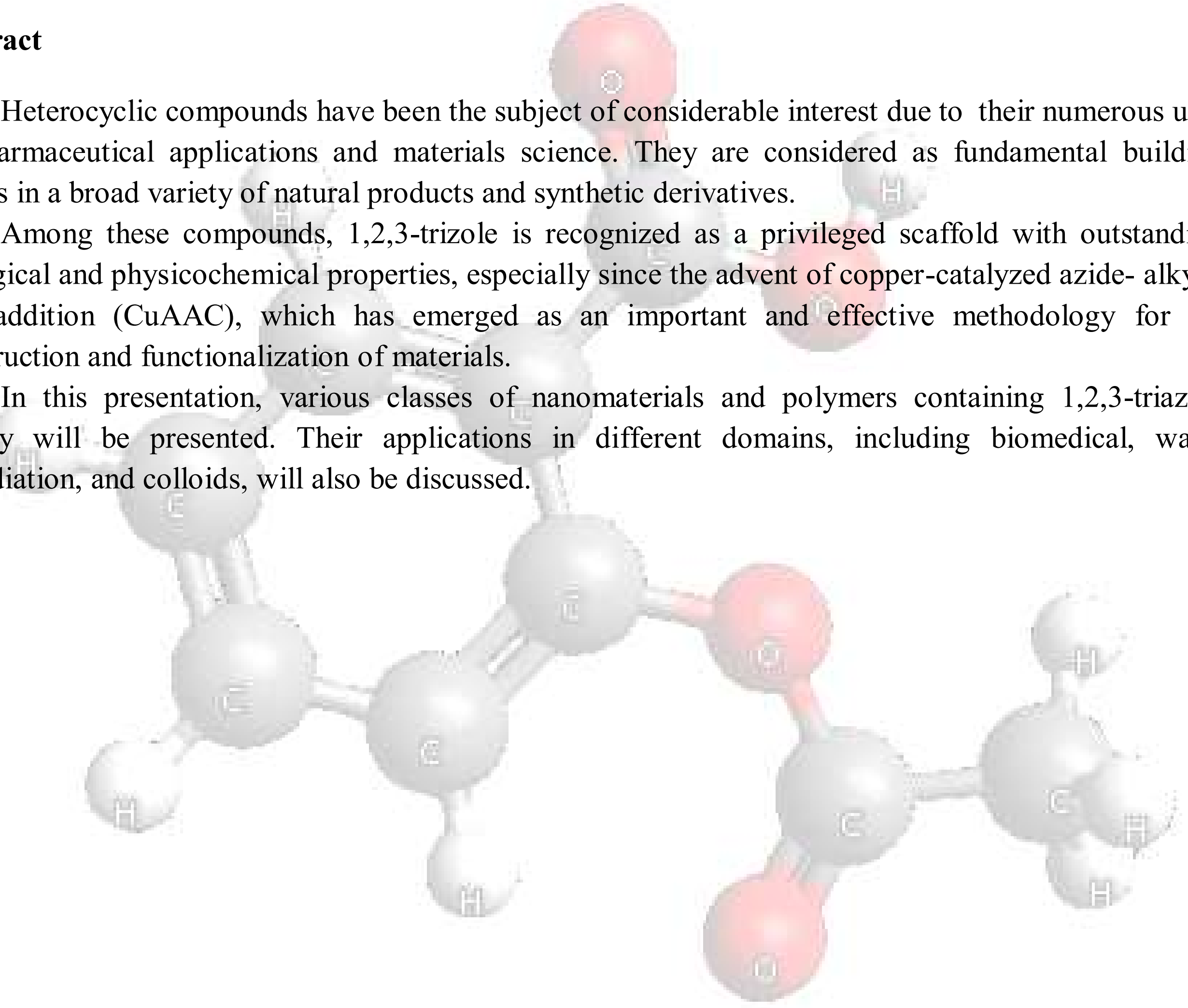
Laboratoire de Synthèse Organique Appliquée, University of Oran 1, Chemistry département, BP 1524 El M'Naoeur
Corresponding Author: saidi.salima@univ-oran1.dz

Abstract

Heterocyclic compounds have been the subject of considerable interest due to their numerous uses in pharmaceutical applications and materials science. They are considered as fundamental building blocks in a broad variety of natural products and synthetic derivatives.

Among these compounds, 1,2,3-trizole is recognized as a privileged scaffold with outstanding biological and physicochemical properties, especially since the advent of copper-catalyzed azide- alkyne cycloaddition (CuAAC), which has emerged as an important and effective methodology for the construction and functionalization of materials.

In this presentation, various classes of nanomaterials and polymers containing 1,2,3-triazole moiety will be presented. Their applications in different domains, including biomedical, water remediation, and colloids, will also be discussed.



NANOMATERIALS: FROM SCIENCE FICTION TO REALITY

Pr. BENACHOUR Djafer

LMPMP, Institut des Sciences et Techniques des MatériauxUniversité Ferhat ABBAS, SETIF
Corresponding Author: bendjafer@univ-setif.dz

Abstract

History of "Nanotechnology": The story of "Nanotechnology" began on December 29, 1959 when Richard Feynman (Nobel Prize in Physics, 1965) pronounced his famous phrase "*There is plenty of room at the bottom*". Through such a phrase, he not only addressed a clear invitation to his fellow physicists to enter a new field of physics, but he also opened the door for new and exciting Sciences and Technologies, i.e. "Nanotechnology". Within the following three decades, the manipulation of matter on an atomic molecular scale became possible (discovery of the Atomic Force Microscope in 1986; atomic writing of the IBM logo in 1989; in 1974, the term "nanotechnology" was first used by Taniguchi on ion-sputter machine, and in 1981 appeared the first technical paper on "molecular engineering" to build with atomic precision…). This novel technology allowed the design and fabrication of new materials at the nanoscale: "nanomaterials" became available in the 1990's.

LES LIQUIDES IONIQUES, PROPRIETES ET APPLICATIONS.

Dr. Taqiyeddine MOUMENE

Laboratoire de synthèse et catalyse Tiaret, université Ibn khaldoun-Tiaret.
Corresponding Author: taqiyeddine.moumene@univ-tiaret.dz

Résumé

La chimie verte implique l'utilisation de principes pour réduire et éliminer l'utilisation ou la génération de substances nocives pour l'environnement, grâce à de nouveaux procédés chimiques et à des voies de synthèse propres, c'est-à-dire respectueuses de l'environnement.

La plupart des solvants organiques sont toxiques et cancérigènes, et certains sont inflammables et dangereux à transporter et à manipuler. Les chimistes recherchent des solvants alternatifs, qui seraient aussi efficaces que les solvants organiques, et qui n'auraient pas les mêmes inconvénients. Ils ont découvert une nouvelle classe de solvants, moins polluants et moins volatils: les liquides ioniques. Les liquides ioniques sont constitués d'un cation le plus souvent organique, associé à un anion organique ou minéral, et les combinaisons cation / anion possibles sont très nombreuses. Les liquides ioniques (LIs) sont des sels liquides qui diffèrent de tous les sels fondus par un point de fusion inférieur à 100 °C. Les liquides ioniques présentent des avantages évidents du point de vue de l'ingénierie des procédés, en raison d'une large gamme de stabilité thermique et chimique, d'une conductivité thermique élevée et d'une faible pression de vapeur. Certains LIs sont totalement non volatils jusqu'à leurs températures de décomposition (généralement supérieures à 300 ° C). Les liquides ioniques présentent ainsi un risque considérablement réduit de rejet accidentel de vapeurs dans l'atmosphère. De plus, la possibilité d'ajuster leurs caractéristiques physico-chimiques en faisant varier la nature de l'anion ou du cation ou en modifiant les substituants portés par le cation de LI, ce qui est un avantage majeur. Il convient également de mentionner que les LIs sont capables de dissoudre un grand nombre de composés organiques ou minéraux.

MOLECULAR SIMULATION IN PHYSICAL CHEMISTRY OF MATERIALS

Pr. ZANOUN Abdelouahab

École Nationale Supérieure d'Enseignement Technologique d'Oran
Corresponding Author: zanounabdelouahab@gmail.com

Abstract

Molecular simulation appeared in the middle of the 20th century. It is a tool widely used to help interpret and understand experimental results, test new theories, or predict the physical or chemical behavior of matter. These “digital experiments” represent a new way of exploring matter, thus complementing theories and experiments in many fields of chemistry, physics and biology.

Molecular simulation methods solve, in a numerical way, the equations of classical and quantum mechanics and statistical thermodynamics, which makes it possible to make the link between the microscopic quantities of the system (such as the positions and speeds of the atoms) and its properties macroscopic (structural or dynamic).

In this contribution, we will present a general overview of the history of atomic reality followed by a reminder of the theory which allows the study of atoms and the principles of molecular simulation with its evolution over time. Some examples relating to molecular simulations will be discussed.

Simulation moléculaire en physico-chimie des matériaux

Résumé

La simulation moléculaire est apparue au milieu du 20ème siècle. C’est un outil largement utilisé pour aider à interpréter et comprendre des résultats expérimentaux, tester de nouvelles théories, ou prédire le comportement physique ou chimique de la matière. Ces « expériences numériques » représentent une nouvelle voie d’exploration de la matière, complétant ainsi les théories et les expériences, dans de nombreux domaines de la chimie, la physique et la biologie.

Les méthodes de simulation moléculaire résolvent, de façon numérique, les équations de la mécanique classique et quantique et de la thermodynamique statistique, ce qui permet de faire le lien entre les grandeurs microscopiques du système (comme les positions et vitesses des atomes) et ses propriétés macroscopiques (structurales ou dynamiques).

Dans cette contribution, nous présenterons un aperçu général sur l’historique de la réalité atomique. Suivi par un rappel de la théorie qui permet l’étude des atomes Les principes de la simulation moléculaire et son évolution à travers le temps. Quelques exemples portant sur des simulations moléculaires seront discutés.

STRUCTURE-PROPERTIES RELATIONSHIP OF FUNCTIONAL MATERIALS: EXPERIMENTAL ANDTHEORETICAL APPROACHES

Pr. CHOUAIH Abdelkader

Laboratoire de Technologie et Propriétés du Solide (LTPS), département de génie des procédés, Faculté des Sciences et de la Technologie, Université Abdelhamid Ibn Badis – Mostaganem, 27000 Mostaganem, Algérie.

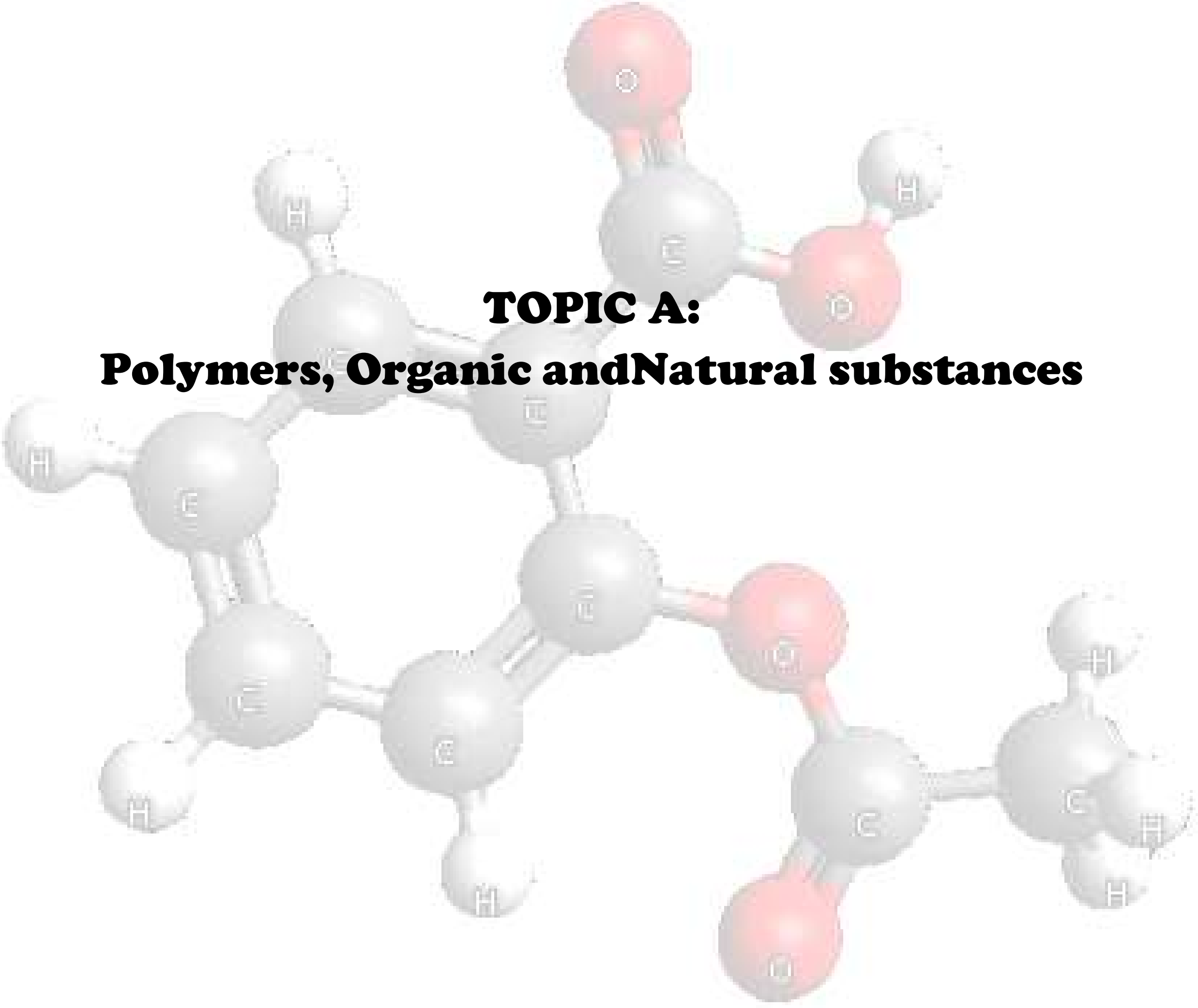
Corresponding Author: achouaih@gmail.com

Abstract

Structure–property relationships have long been considered important explanatory concepts in the disciplines of chemistry, physics and biology to study functional materials. Experimental and computational methods have played an important role in discovering their properties. However, the theoretical approaches range from very empirical schemes to abs initio methods that require no experimental data. In some cases, predictions of new advanced materials were made and subsequently confirmed by measurements. Researchers are thus in the early stages of using theory and computation to "design" functional materials. Among them, heterocyclic compounds are considered the most important classes of organic compounds that have attracted much attention for their various activities. Knowledge of the crystal structures of these compounds is crucial for understanding the related activity. In this communication, we will focus on the different properties of functional materials that can be investigated theoretically and experimentally.

Keywords: Advanced materials, X-ray structure, theoretical calculations, reactivity.

TOPIC A:
Polymers, Organic andNatural substances



GREEN CHEMISTRY APPROACH FOR DESIGNING ENERGETICPOLYBENZOXAZINES: VANILLIN AS A SUSTAINABLE PRECURSOR

Slimane ABDOUS[*,1], Mehdi DERRADJI[1], Karim KHIARI[1], Oussama MEHELLI[1], Noureddine RAMDANI[1], Abdeljalil ZEGAOUI[1], Wenbin LIU[2]

[1]UER Procédés Energétiques, Ecole Militaire Polytechnique, BP 17, Bordj El-Bahri, Algies, Alegria,
[2]Institute of Composite Materials, Key Laboratory of Superlight Material and Surface Technology of Ministry of Education, College of Materials Science and Chemical Engineering,Harbin Engineering University, Harbin 150001, China
Corresponding Author: slimane.abdous.emp@gmail.com

Abstract

This study introduces a new group of environmentally friendly benzoxazine polymers with high energy content, using vanillin as a sustainable starting material. The novel monomers were obtained through the reaction of vanillin with the energetic precursor compounds: 2-4 dinitrophenylhydrazine and para-nitroaniline, following the conventional Mannich reaction. The mechanism of ring opening polymerization was investigated using FTIR and DSC-TGA analyses. The energetic performance and physico-chemical properties of the polymers were evaluated using bomb calorimetry, deflagration testing, and electronic densimeter. Overall, the results demonstrated promising energetic performances for both polymers, with deflagration temperatures of approximately 275°C and 261°C for the 2-4 dinitrophenylhydrazine and para-nitroaniline-based polybenzoxazines, respectively. Furthermore, the combustion heat released during their deflagration was significantly higher compared to commonly used energetic polymers such as nitrocellulose and diol-glycide-azide polymers. Thermal analysis indicatedthat these polymers exhibit both rigidity at operational temperatures and remarkable energetic properties, making them suitable for applications as reactive structure materials (RSMs).

Keywords: Benzoxazine, Mannich reaction, Energetic monomer, Explosophore groups, Vanillin.

THE STUDY OF THE INHIBITION EFFICIENCY OF GREEN INHIBITORS ON API 5L-X52 STEEL

Mohammed SADOU[*,1] **& Mohamed HADJMELIANI**[2]

[1] *Laboratory of Materials, Catalysis and Reactivity Chemistry (LCMCR), Hassiba Benbouali University of Chlef, B.O. Box 151, Chlef 02000. Algeria.*
[2] *LPTPM, Hassiba Ben Bouali University of Chlef, B.O. Box 151, Chlef 02000., Algeria.*
Corresponding Author: m.sadou@univ-chlef.dz

Abstract

Corrosion is the natural electrochemical process in which refined metals are converted into more stable compounds such as metal oxides, metal sulfides, or metal hydroxides through oxidation and deterioration, causing a great damage in industry, the use of inhibitors is one of the most common methods of protecting metals against corrosion, but the search for eco-friendly corrosion inhibitors is still continuous due to differences in corrosive media and it remains an important point in corrosion control. This work presents a study conducted in the field of corrosion inhibition of steel in a 1 M hydrochloric acid (HCl) environment using novel inhibitors derived from plant extract, additionally, the influence of inhibitor concentration, immersion time, and temperature on the inhibition efficiency was investigated. The study provides valuable insights into the performance of green inhibitors as environmentally friendly alternatives for corrosion protection of API 5L-X52 Steel in HCl environments.

Keywords: Corrosion, Calotropis Procera, Datura Stramonium, Green inhibitor, API 5L-X52

PREPARATION AND CHARACTERIZATION OF NATURAL POLYMER AND ITS USE

Hafida ZERGUI*,1, Fatima HABECHE[2], Rachid MEGHABAR[3], Fatima ZEGGAI[4]

[1] *Department of chemistry, Faculty o exact and applied sciences, University of Oran1, 31000,Oran, Algeria,*
[1,3]*University of Oran1 Ahmed Ben Bella, Oran, Algeria*
[2]*University of Sciences and Technology Mohamed Boudiaf, Oran, Algeria*
[4]*Center for Scientific and Technical Research in Physico-Chemical Analysis*
Corresponding Author: zeriguihafida@gmailcom

Abstract

Alginates are polysaccharides considered as biopolymers, extracted mainly from brown algae. They are widely used in various fields and many industries because of their biocompatibility and biodegradability.

In recent years, alginate hydrogels in the presence of divalent or trivalent cations (Ca^{2+}, Ba^{2+}, Pb^{2+}, Ti^{2+}, Fe^{3+}, Al^{3+}) have attracted many researchers due to its amazing properties and its medical and biomedical applications, as an active ingredient in skin dressings or as excipients. In this paper, we propose a method for the synthesis of alginate hydrogels « divalent and trivalent cations » in different concentrations using the sonicator. This ultrasound ensures good agitation between the molecules with possible speed adjustment. After that we dried hydrogels by two different methods (freeze dryer and oven). this allows us to make acomparative study between iron and titanium, the concentration of metals, and the difference between the use of the oven and the freeze dryer and their influence on the hydrogels using different methods of analysis: X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy and Differential scanning calorimetry (DSC).Finally, to reinforce the work we have done on the treatment of water by adsorption to study the effect of each sample.

Keywords: Biopolymer, Alginate, Metals, Hydrogel, Ultrasound.

STUDY OF THE COMPLEXATION OF TETRACAINE ANDLIDOCAINE HYDROCHLORIDE IN CYCLODEXTRINS IN THE SOLIDSTATE

F. CHATER, T. FERGOUG, C. ZELMAT, F. YASSAD, Y. BOUHADDA.

Laboratory of Physical Chemistry of Biomolecules and Biological Interfaces, University ofMascara, Mascara 29000, Algeria
Corresponding Author: f_chater@yahoo.fr

Abstract

La formulation d'un médicament à l'état solide repose sur un bon synergisme entre le principe actif et l'excipient utilisé. Ce synergisme est d'autant plus important que les deux molécules forment un complexe stable à l'état solide. Le but de cette étude est de confirmer la formation de complexes d'inclusion entre deux molécules anesthésiantes la Tétracaine (TC) et la Lidocaine hydrochloride (Lid,HCl) avec deux types d'excipient cyclodextrines CD (βCD et HPβCD). Deux méthodes de préparation ont été adoptées, la première consiste en la préparation par pétrissage « kneading » et la seconde par co-évaporation en présence de différents solvants. La mise en évidence du complexe a été établit expérimentalement au moyen de la calorimétrie différentielle à balayage (DSC). A partir des différents thermogrammes les températures de fusion des complexes formés ont été déterminées et les énergies de complexation déduites. Autres caractéristiques comme les températures de cristallisation et vitreuses ont été détectées pour certains complexes. En comparant les méthodes de préparation adoptées dans cette étude onconclut que les méthodes de pétrissage « kneading » et de co-évaporation permettent une meilleure encapsulation du principe actif, comparées à la méthode de co-évaporation en présence des deux solvants éthanol et chloroforme.

Keywords : Tétracaine (TT), Lidocaine hydrochloride (Lid,HCl), complexe d'inclusion, DSC

EXPERIMENTAL STUDY OF MECHANICAL AND THERMAL BEHAVIOR OF POLYVINYL ALCOHOL FIBER ON THE CEMENT

Benamar BAROUDI[*,1], **Leila DJAHNIT**[2,3], **Mohammed TEHAR**[3], **Nadia LAKREB**[4,5]

[1] Laboratory of Organic Chemistry, Macromolecular and Materials, Department of Chemistry, University Mustapha Stambuli of Mascara, BP 763, 29000 Mascara, Algeria
[2] Physico-Chemistry of High Polymer Laboratory Ferhat Abbes University of Setif, Algeria
[3] Department of chemistry, faculty of exact sciences and informatics, University Hassiba Benbouali, Chlef, Algeria
[4] Research Unit Materials, Processes and Environment, University M'Hamed Bougara, Boumerdes, Algeria
[5] Departement of Materials Sciences, University of Science and Technology Houari Boumediene, Bab Ezzouar, Algeria
Corresponding Author: benamarbaroudi@gmail.com

Abstract

The development of polymer-mortar composites, originates from certain needs expressed by building and public works professionals. These materials are most often used in secondary work such as facade coatings, adhesive tiles or sealing coatings; they are also used in the field of public works as repair products for works of art, and in certain road applications. In the end, we are looking for a simple implementation material, with a better holding in service compared to a standard mortar. It must also have good adhesion properties as well as increased resistance to environmental aggressions and in particular insulation from walls to moisture. The durability of concrete structures is a very important feature because it is the guarantee of increased safety and service life of these structures. This durability also guarantees a considerable economy in the long term, because such works will require little or no repair, hence a cost savings induced by repairs, which can be very high, and may even exceed the costs Initial construction. In order to apprehend the influence of the polymer on the mechanical behavior of Cement materials composites based on different levels of polyvinyl alcohol (PVA) have been carried out, which we have conducted mechanical tests such as Resistance to compression and traction by bending three points and Physico-chemical tests such as standardized consistency, expansion and measure heat hydration. This research indicates that PVA can provide effective reinforcements in cement-matrix composite materials and can be used in various applications

Keywords: cement, PVA, bending, Compression, expansion, heat of hydration

IN VIVO AND *IN SILICO* TOPICAL ANTI-INFLAMMATORYPROPERTIES OF PHYTOCHEMICALS AND PLANT-DERIVED ESSENTIAL OILS: A COMPREHENSIVE REVIEW

B.S. BOUKHATEM[*,1], A.E. BELHADJ

[*] *Laboratory of Biomaterials and Transport Phenomena, Faculty of Technology, University of Médéa, Algeria*
Corresponding Author: boukhatem.bouchra.sarah@gmail.com

Abstract

Topical inflammation is a physiological reaction to a variety of agents such as bacterial and fungal infections, dangerous chemicals and reagents, and physical injury. Skin inflammation, autoimmune diseases, and cancer are all linked with the progression of inflammation. Nonsteroidal anti-inflammatory drugs (NSAIDs) and corticosteroids are two treatments that can be used to suppress or reduce the inflammatory process, but they both have a wide range of adverse effects disturbing the gastrointestinal membrane, renal structure, cardiovascular, hepatic and blood systems. Phytotherapy, herbal medicines and aromatic plants have long been used to meet the health needs of the population, and they now provide a wide variety of healthcare options and health-benefits. The search for alternative NSAIDs capable of interrupting the inflammatory process has emerged as an important topic in scientific research, especially in terms of natural product application and the reduction of systemic adverse effects. Because their active components have a variety of biological effects, including anti-inflammatory activity, phytochemicals and plant-derived essential oils (EOs) are useful source of these bioactive compounds. Plant-derived EOs analysis and application have grown in importance in scientific research and industrial processes in recent years, including medicinal, pharmaceutical, nutritional, and cosmetic applications. This presentation provides an overview of the *in vivo* and *in silico* anti-inflammatory activity of phytochemicals and terpenes derived from EOs, as well as a discussion of potential modes of action related to the anti-inflammatory response, as evaluated using different experimental models.

Keywords: Phytochemicals, Plant-derived essential oils, Oxygenated terpenes; Topical anti-inflammatory activity; Histological examination.

SYNTHESIS AND CHARACTERIZATION OF NEW ANTIMICROBIAL, ANTI-INFLAMMATORY, AND ANTIFUNGALCOMPOUNDS BASED ON SCHIFF BASE LIGAND

Raziqa DJAAFER MOUSSA[*,1], Leila DJAHNIT[2], Rachid DELLAI[3], Wafa LAMIRI[1], Fatima SETIFI[1], Lakhemici KABOUB[1]

[1] Laboratoire De Chimie, Ingénierie Moléculaire Et Nanostructures, Département De Chimie,Faculté Des Sciences, Université Ferhat Abbas Sétif-1, 19000, Sétif, Algérie.

[2] Département De Chimie, Faculté des Sciences Exactes et Informatique, Université Hassiba BenBouali, Chlef, Algérie

[3] Laboratoire de Recherche Sciences et Environnement (SCIENV-C1810200), département dechimie, faculté des sciences et technologies, Université Amine El Okkal El Hadj Moussa Eg Akhamouk de Tamanghasset, sersouf 11000 Tamanghasset, Algérie

Corresponding Author: raziqa.djaafermoussa@univ-sétif.dz

Abstract

It is well known that several Schiff base complexes of Ni(II), Cu(II) and Zn(II) are used as anti-inflammatory, antipyretic, chemosensor, anti-diabetic, anti-bacterial, anti-cancer and anti-HIV (HIV virus). human immunodeficiency). In this work, we synthesized a new 4-[(2-hydroxy-3- methoxy-benzylidene)-amino] butanoic acid Schiff base ligand, by the condensation reaction of 2-hydroxy-3-methoxy benzaldehyde and l 4-amino butanoic acid in absolute ethanol. The complexes were obtained by the coordination of the ligand with the metal salt, the compounds synthesized and characterized by IR, UV-vis, and the electrochemical study by cyclic voltammetry aims to study their redox properties. The in vitro antimicrobial effects of the synthesized compound were tested against eight bacterial species and a single fungal species by the well diffusion method. The results of the anti-inflammatory activity thus make it possible to conclude that the ligand and the two Cu (II) complexes L and Mn(II)L have acceptable protein denaturation inhibitions compared to the reference anti-inflammatory (aspirin). Metal complexes show more biological activity than Schiff's base.

Keywords: Schiff base, antifungal activity, anti-inflammatory activity, cyclic voltammetry, coordination complex.

THEORETICAL STUDY OF THE EFFECT OF THE PLANT AND SYNTHETIC FIBERSON THE FIBER-MATRIX INTERFACE DAMAGE OF BIOCOMPOSITE MATERIALS BASED ON PHAS (POLYHYDROXYALKANOATES) BIODEGRADABLE MATRIX

Naima KAOUCHE

Department of Materials Technology, Faculty of Physics, Faculty of Physics, University of Science and technology, USTO-MB, El Mnaouar, BP 1505, Bir El Djir 31000, Oran, Algeria
Corresponding Author: naimakaouche19@gmail.com

Abstract

The natural plant fibers and biopolymers are a very important alternative to replace the inorganic fibers most used in the mechanical reinforcement of composite materials (carbon, glass, …) and synthetic polymers (Epoxy, PEEK, …), and at the same time they have a very low environmental impact and a very reasonable price. In this article, we have studied, by a numerical simulation based on genetic approach, the fiber-matrix interface damage of composite materials made up from the PHA (polyhydroxyalkanoates) matrix and the carbon, glass, jute, and hemp reinforcements with the same volume fraction equal to 30% for each fiber chosen. Our results showed that the damage at the fiber-matrix interface of the biocomposite hemp/PHA is the lowest compared with the other biocomposite materials glass/PHA, jute/PHA, and carbon/PHA. This finding is similar to that found by Antoine Le Duigou *et al.* and Bodros *et al.*, where they have shown experimentally that the natural reinforcements greatly improve the properties of composite materials and also they have a very low environmental impact. To our knowledge, no published research reports on the study of fiber-matrix interface damage of biocomposite materials based on PHAs and carbon, glass, jute, and hemp fibers for potential textile applications, packaging, and other interesting areas.

Keywords: Biocomposite, Damage, PHA (polyhydroxyalkanoates), Natural plant fibers, Interface

DRUG RELEASE STUDY OF METRONIDAZOLE FROMSIMPLE AND DOUBLE WALLED MICROPHERES

Khalida MECHETTEM*^,1^, Kheira DIAF, Zineb ELBAHRI[2]

[1] *Laboratoire de Chimie Organique Physique et Macromoléculaire, Faculté des SciencesExactes, Université Djillali Liabès de Sidi Bel Abbes22000, Algérie.*

[2] *Laboratoire de Matériaux & Catalyse, Faculté des Sciences Exactes, Université Djillali Liabès de Sidi Bel Abbes, 22000, Algérie.*

Corresponding Author: mechettem.mechettem@yahool.fr

Abstract

The main objective of the present work is to develop delayed release polymeric formulations loaded by metronidazole. This active ingredient is an antibacterial, anti-parasitic and antibioticand it has a high solubility at pH 1.2. So to attain an efficient *colonic drug delivery* for local or systemic drug effects, the double coating method strategy has been explored.

For the purpose, firstly simple walled microspheres based on ethylcellulose as polymeric matrix are prepared using water in oil emulsion-solvent evaporation technique, the stirring speed was set at 800 rpm. In the second step, the obtained formulations were coated using another biomaterial and using hot-meltprocess of microencapsulation.

The obtained formulations are characterized by infrared spectroscopy and X-Ray diffraction analysis and the size distribution of microparticles is determined by the optical microscopy.

The drug release is studied in a simulated gastric liquid at pH=1.2 at 37°C and an intestinal medium (pH=6.8) and analyzed using UV-Vis spectrophotometer.

The drug loading was 37% and 4% in simple and double coated microspheres respectively. The results demonstrated that metronidazole release was largely slowed down using this approach and so promising colon targeted drug delivery systems can be obtained.

Keywords: Metronidazole, double coated microspheres, biomaterial, drug release.

EPSs of EXTREMOPHILIC BACTERIA AND THEIRAPPLICATIONS IN THE FOOD INDUSTRY

Nadjette MOUMENE*,1, Wafa MALKI[1], Khalid ACHERRAT[1], Mounia ARAB[1,2], Amine MESLI[1], Nihel KHELIL[1]

[1]Laboratory of Applied Microbiology in Food, Biomedical and Environment, Department ofBiology, Faculty of Nature Sciences and Life, University of Tlemcen, Tlemcen 13000.
[2]Faculty of Biological Sciences, University of Sciences and Technology Houari Boumediene, Algiers.
nadjetmoumene@gmail.com.

Abstract

Exopolysaccharides (EPSs) are one of biopolymers produced by bacterial communitiesto strive various extreme environmental conditions.

These biomolecules are extracellular carbohydrate biopolymers secreted by microorganisms, which accumulate outside cells, they are able to be released into the surrounding environment. EPSs produced by extremophiles have attracted potential research interest for several biotechnological applications due to their good thermal stability, non-toxicity and biodegradability.

For example, food industries around the world are looking for value-added compoundsor additives of natural origin with increased functionality and bioactivity. In addition, a growing trend can currently be observed among the consumer towards healthier foods. This communication aims to give an overview about the potential applications of bacterial EPSs.

Isolation of bacterial strains was carried out by plating the serially diluted water samples on nutrient agar followed by incubation for 24 to 48 h, then screened for EPS production based on slimy appearance of their colonies. The selected colonies were inoculated in a nutrient broth for EPS quantification, which were then extracted, purified and characterized based on their phenotypique characteristics for use in further studies.

The functional properties of EPSs were evaluated for food industry applications.

EPSs play an important role in improving the rheological and sensory characteristics of food products by positively influencing food texture and organoleptic properties. Moreover, these biomolecules have been considered as promising antioxidants for developing effective functional foods with longer shelf life. Furthermore, EPSs possessing water and oil retaining capabilities are also exploited to prepare functional food products by stabilizing water and oil emulsions.

In conclusion, we can deduce that EPSs are promising candidates that can be used as useful additives for the food industry. Thus, the production and characterization of extremophilic bacterial EPS is an active area of research to improve culture techniques,in a cost-effective manner.

Keywords: Exopolysaccharides, Biopolymers, Extremophiles, Food industries.

SYNTHESIS, CHARACTERIZATION AND ELECTROCHEMICAL PROPERTIES OF V_2O_5 NANOPARTICLESINTERCALATED WITH PANI-DERIVED

Mounya ZENASNI[*,1,3], **Cherifa Hakima MEMOU**[2], **Abdelghani BENYOUCEF**[3]

[1] *Department of Electrical Engineering, Faculty of Electrical Engineering, University Djillali Liabes, Sidi Bel Abbès, Algeria.*
[2] *Laboratory of Physical and Macromolecular Organic Chemistry; Faculty of Exact Sciences;Djillali Liabes University, Sidi Bel Abbes, 22000, Algeria.*
[3] *LSTE Laboratory, University of Mustapha Stambouli Mascara, 29000, Algeria.*
Corresponding Author: zenasni_mounya@yahoo.fr

Abstract

Hybrid materials consisting of aniline (ANI) and/or 2-aminodiphenylamine (2ADPA) in the presence of V_2O_5 nanoparticles were synthesized by in-situ chemical oxidative polymerization in the presence of ammonium persulfate as an oxidant. The synthesized nanocomposites were characterized using XPS, FT-IR, XRD, XRF and UV-vis techniques. Structural and morphological investigations confirmed the presence of polymer and V_2O_5 nanoparticles, which were in interaction in the nanocomposites. The XRD patterns indicated that morphology of P(2ADPA)/V_2O_5 and poly(ANI-co-2ADPA)/V_2O_5 is crystal structure and it is different from PANI/V_2O_5. The optical properties are studied. The optical band gap of materials found to increase in the following order: PANI/V_2O_5< poly(ANI-co-2ADPA)/V_2O_5< P(2ADPA)/V_2O_5, i.e. with the content of ANI monomer. Thermal stability of the composites is determined using TGA analysis. The morphology of the samples is studied using SEM. The electrochemical properties were investigated by cyclic voltammetry to explore the advantages of these samples for potential applications. These results highlight the great influence of the V_2O_5 interface and the nature of monomer on the hybrid materials formation and properties.

Keywords: Aniline; 2-aminodiphenylamine; Vanadium Oxide; Nanocomposites, Electrochemical properties.

ADSORPTION OF CRYSTAL VIOLET: PARAMETEROPTIMIZATION AND KINETICS ANALYSIS

Kelthoum SAADALLAH, Chifaa AD, Mebrouk DJEDID, Mokhtar BEALIA, Romaissa HADJ AISSA

Department of process engineering, Faculty of Technology, University of Laghouat., 03000,Laghouat, Algeria, Laboratory of process engineering

Corresponding Author: k.saadallah@lagh-univ.dz / kelthoumsaad25@gmail.com

Abstract

Industrial effluent streams have been reported to contain dyes as initial pollutants. These substances pose significant threats to human health and aquatic ecosystems. Due to its mutagenic and carcinogenic properties, crystal violet (CV), a widely used synthetic dye, is considered hazardous. In order to mitigate this problem, we have employed pea peels powder as an effective adsorbent to eliminate crystal violet (CV) dye from synthetic water. We optimized the experimental parameters in a batch technique to investigate the impact of various factors on dye exclusion, including adsorbent dosage, pH, contact time, dye concentration, and temperature. We used the pseudo-first-order and pseudo-second-order models to assess the reaction kinetics. At the ideal conditions, the dye removal effectiveness reached its maximum, eliminating 87.47% of the dye. The experimental settings involved an adsorbent dosage of 0.6 g, a temperature of 55°C, a pH of 7, a dye concentration of 150 ppm, and a contact time of 60 minutes. The kinetic analysis findings indicate that the pseudo-second-order kinetics model can accurately describe the observed process. Successful demonstrations of this approach with synthetic water provide evidence to support the effectiveness of green pea peels as a locally available and cost-effective adsorbent to decontaminate synthetic water from dyestuff.

Keywords: adsorption, crystal violet, pea peels, optimal parameters, kinetics.

CONTRIBUTION TO THE STUDY OF THE THERMAL PROPERTIES OFPLA/PMMA BLENDS

Lynda ABBANE, Naima KHEMICI-DOULACHE, Mohamed Wafik KHEMICI

Department of Physics, Faculty of Physics, University of Science and Technology HouariBoumediene (USTHB), 16111, Bab-Ezzouar, Algeria

Corresponding Author: labbane@usthb.dz

Abstract

In this study, we focused on investigating the thermal properties of PLA/PMMA (Poly (lactic acid)/Poly (methyl methacrylate)) blends through enthalpy measurements using DSC (Differential Scanning Calorimetry). To achieve this, we prepared several samples with varying mass fractions of PMMA, specifically 0%, 10%, 20%, and 30%, using the solvation method. Subsequently, we recorded DSC thermograms over a temperature range from -10°C to 300°C, revealing the appearance of amelting peak at around 148°C and a characteristic endothermic jump corresponding to the glass transition at about 50°C. The uniqueness of these features in each sample indicates that the PLA/PMMA blend is miscible. Furthermore, weobserved a decrease in the melting temperature with saturation for high mass fractions of PMMA. Regarding the glass transition temperature, it remained close to that of PLA, indicating no significant changes. From a calorimetric perspective, we were able to calculate the fusion enthalpies and heat capacity of our samples, with some approximations made. Specifically, we assumed that the fusion enthalpy of the completely crystalline blend is identical to that of pure PLA. As for the heat capacity of the blend, we derived an empirical formula by analogy with the one used for calculating the glass transition temperature of a blend. Using the values obtained and applying the three-phase model that governs phases in a polyester, we estimatedthe degrees of crystallinity in our blends, as well as the proportions of the mobile amorphous phase and the rigid amorphous phase. The main observations revealed an increase in both the crystalline and rigid amorphous phases at the expense of the mobile amorphous phase as the PMMA fraction increased.

Keywords: PLA, PMMA, Differential Scanning Calorimetry (DSC), solvatation method, miscibility.

CRAMAN SPECTROSCOPY CHARACTERIZATION OF ECO-FRIENDLY NANOCOMPOSITES BASED ON POLY(Ɛ-CAPROLACTONE)MODIFIED WITH RECYCLED RED MILL SCALE

Rachid DELLALI[*,1], Leila DJAHNIT[2,3], Samira MAOU[2], Saida SOUALMI[4], Khaled El-MILOUDI[5], Mazouri BENNAMA[2], Abdelyamine NAITBOUDA[6]

[1]Laboratory of scientific research sciences & Environment SCIENV-C1810200, Department ofscience of the matter (chemistry), Faculty of sciences and Technology, University Amine El okkal El Hadj Moussa Eg Akhamouk Of Tamanghasset, sersouf 11000 Tamanghasset, Algeria
[2]Chemistry department .Faculty of exact sciences and informatics, Hassiba Benbouali University(UHBC) Chlef Algeria,
[3]Renewable Energy and Materials Laboratory, Medea University
[4]Laboratory of synthesis and Catalysis, University of Tiaret
[5]Faculty of Technology, Hassiba Benbouali University (UHBC) Chlef Algeria
[6]Advanced Technology Development Center
Corresponding Author: rachidcvp86@gmail.com

Abstract

Recycled Red Mill Scale (RS) particles are a waste product of the iron and steel industry, and they are magnetic and consist mainly of iron oxides (Fe_2O_3, Fe_3O_4) with improved permittivity. They can be reinforced with non-conductive polymer matrices such as poly-caprolactone (PCL), which is easily mixed with metal oxides to make absorbers with promising properties. In this work, recycled red mill-scale particles were decreased to nanosize using ultrasoundirradiation. Using the solution-blend process, a total of 1–20 wt.% recycled nanofiller loadings were integrated into a red mill scale/non-conducting PCL polymer matrix to construct film nanocomposites. In the first investigation, we are looking at Raman Spectroscopy characterization.

PCL matrix and its modifications following the RS particle integration for three spectral ranges: 1150-1000, 1770-1700, 1380-1200 cm^{-1}, which depicts the peak fit models and findings for the individual spectral ranges. The comparatively high standard deviation values, particularly for the PCL/RS film, demonstrate the heterogeneous nature of the nanocomposites and the amorphousness increases widely with the inclusion of RS in all nanocomposites, especially at 20%. In the three areas mentioned above.

Keywords: polymer nanocomposites; PCL; Recycled Red Mill Scale, Raman Spectroscopy; crystallinity.

STUDY OF THE BEHAVIOR OF COPPER WITH RESPECT TO THE SYNTHESIS OF FURAN HETEROCYCLES AS WELL AS THEIRBIOLOGICAL ACTIVITIES

Samira Hamza REGUIG* & Ghenia BENTABED-ABABSA

Laboratory of Applied Organic Synthesis, Faculty of Exact and Applied Sciences, University ofOran 1, 31000, Algeria.
Higher normal school of Oran (E.N.S.O)
Corresponding Author: hr.samira@yahoo.fr

Abstract

Heterocyclic molecules play a very important role in life processes and are of major interest in industrial development in the field of dyes, pharmaceuticals, natural products, etc.

In previous work, several heterocycls were synthesized by 1, 3-dipole cycloaddition using the dipole *gem*-dicyanoepoxids.

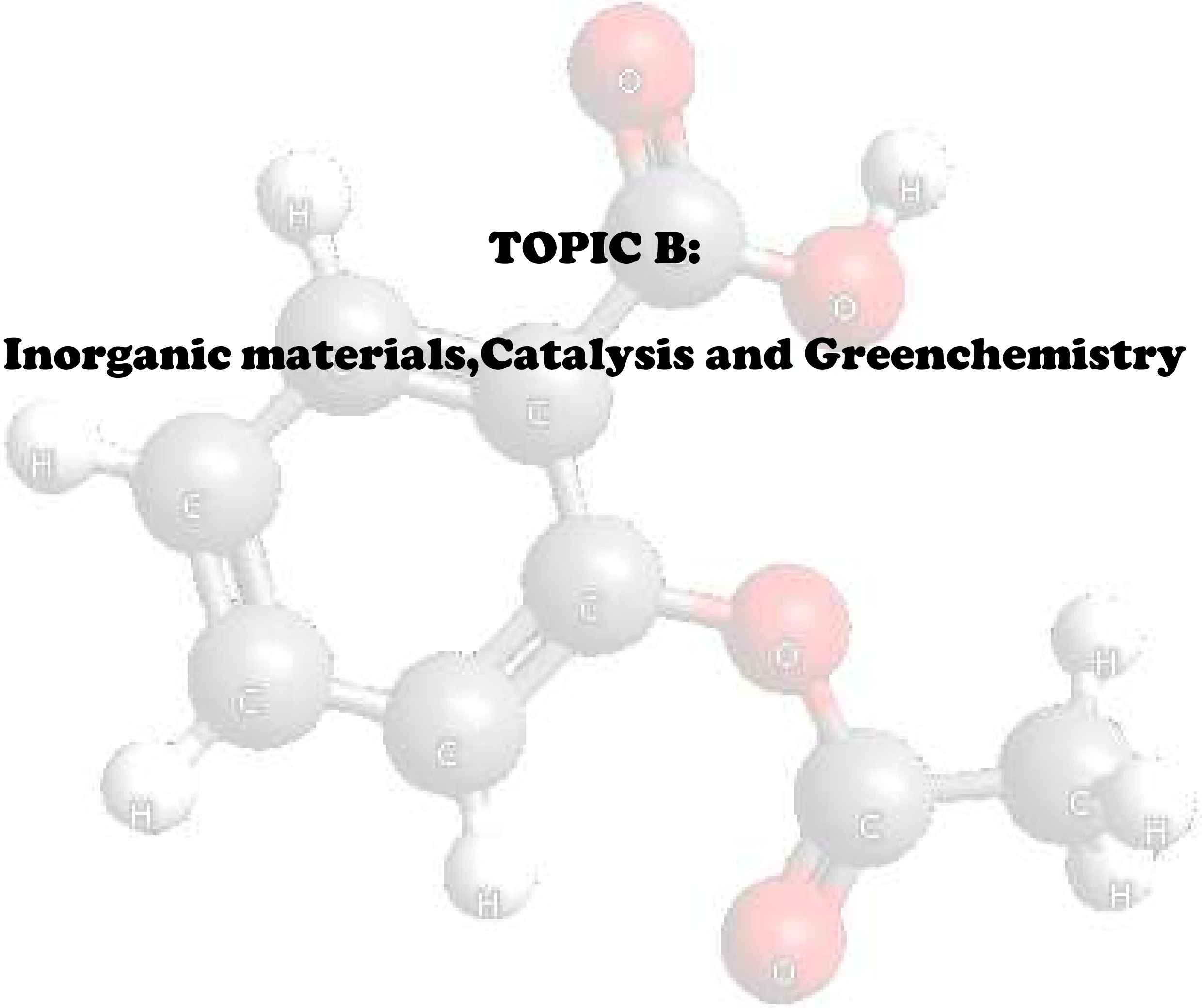
For our part, we have set ourselves the objective of synthesizing a family of heterocycles of the tetrahydrofuran and dihydrofuran type, by the use of *gem*-dicyanoepoxids as dipole, and various alkenes and alkynes. To achieve this, we have chosen heating in the presence and absence of CuII as a catalyst. A comparative study has been established, and the use of catalysis has allowed us to improve yields and reduce reaction times compared to the conventional method without catalyst.

In vitro tests on their antimicrobial and cytotoxic activities (IC50) have been done. The results are comparable, promising and highly effective compared to the chosen controls.

Keywords: *gem*-dicyanoepoxids, 1, 3-dipolar cycloaddition, dihydrofuran, tetrahydrofuran, catalyst.

TOPIC B:

Inorganic materials,Catalysis and Greenchemistry



REMOVAL OF METHYL GREEN BY AN ALGERIANCALCIC CLAY

Imene FEDDAL[*,1], **Youssra BOUMEDIENE**[2], **Goussem MIMANNE**[3]

[1] *Abdel Hamid Ibn Badis University of Mostaganem 27000, Algeria*
[2] *Djillali Liabes University of Sidi Bel Abbes 22000, Algeria*
[3] *Laboratory of Materials & Catalysis, Faculty of Exact Sciences Djillali LIABES University (UDL)*
Corresponding Author: fimene22@hotmail.com

Abstract

The history of the environment and its chemistry is above all the history of its pollution. For a large part, it is the changes made in the air, water and soil by human beings. From there, we can define that pollution is an unfavorable modification of the natural environment that appears as a by-product of human action, through direct and indirect effects.

The protection and preservation of the environment is one of the pillars of sustainable development, which is currently a major issue for the future of man and the planet. Currently, humanity is facing an alarming increase in the pollution of the natural environment by various organic or inorganic materials.

The objective of our work is to study the adsorption of a textile dye which is known in the industrial environment, methyl green, on raw calcic clay. Our material was characterized byXRD, FTIR, we also determined its CEC, pHzc and specific surface by Methylene Blue method. The kinetic and thermodynamic study of the adsorption of methyl green was studied, theseexperiments resulted that the adsorption of the dye follows pseudo second order kinetics, andaccording to the thermodynamic study and the study of the probability we can say that we have aphysisorption.

Keywords: Calcic clay, Dye, Adsorption, Environment, Material.

SYNTHESIS AND CHARACTERIZATION OF $LaAl_{0.9}Fe_{0.1}O_3$VIA SOL-GEL METHOD

Hamza MEDJADJI[*,1], **Ali BOULAHOUACHE**[1,2], **Nassima SALHI**[1,2]

[1] *Laboratoire LCPMM, Faculté des Sciences, Université BLIDA1, B.P 270, Route de Soumaa, BLIDA, Algérie.*
[2] *Laboratoire de Chimie du Gaz Naturel, Faculté de Chimie, USTHB, BP32, El-Alia, 16111 Bab Ezzouar, Alger, Algérie.*
Corresponding Author: hamzamedjadji1990@gmail.com

Abstract

In this study, a nanostructured ternary oxide perovskite, $LaAlO_3$ partially substituted with iron ($LaAl_{0.9}Fe_{0.1}O_3$) was prepared by sol-gel method using $La(NO_3)_36H_2O$, $Al(NO_3)_39H_2O$, and $Fe(NO_3)_39H_2O$ as raw materials and propionic acid as solvent. The salts previously dehydrated in a desiccator were dissolved in distilled propionic acid and the homogeneous solution was evaporated under stirring until total solvent evaporation. The obtained gel was then calcined in air at 800 °C/4h.

Various techniques were used to investigate the structural and textural properties of the material including TGA-DT, X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), UV-visible spectroscopy, Scanning Electron Microscopy (SEM-EDX) and X-ray Photoelectron Spectroscopy (XPS), photoluminescence (PL). Electrochemical analysis was also undertaken.

The XRD analysis of the prepared powder indicates a pure perovskite phase at 800°C with a Rhombohedral structure with R-3c space group and average crystallite size of 36 nm. Such sizes are closer to nanoscale. SEM analysis revealed an appearance of small grain with semi-spherical morphology. In the SEM-EDX analysis, only La, Al, Fe and O elements were detected, indicating the absence of any other contaminating elements and therefore the purity of the material. The Mott-Schottky curve was employed to carry out the electrochemical analysis, which showed that $LaAl_{0.9}Fe_{0.1}O_3$ is an n-type semiconductor with a flat band potential (Efb) of 0.37v.The direct optical band gap E_g (2.28 eV) was determined from the diffuse reflectance using UV-visible spectroscopy. The Xps analysis showed an enery conduction band ECB of 3.25eV. Spectroscopy FT-IR analysis showed characteristic bands of $LaAl_{0.9}Fe_{0.1}O_3$ at 652 cm^{-1} and 420 cm^{-1}.

Keywords: $LaAl_{0.9}Fe_{0.1}O_3$, Perovskite, Sol-gel, Synthesis, Characterization

ADSORPTION OF METHYL ORANGE BY MODIFIEDMONTMORILLONITE

Houria REZALA* & **Naoual TIDJANI**

Department of Technology, Faculty of Sciences and Technology, Djillali Bounaama of Khemis-Miliana University, 44001, Khemis-Miliana, Algeria

Corresponding Author: h.rezala@univ-dbkm.dz

Abstract

Clays intercalated with cetyltrimethylammonium bromide and/or hydroxy aluminum polycation were prepared and analysed by X-ray fluorescence spectrometry, X-ray diffraction, Fourier transform infrared spectroscopy, nitrogen adsorption-desorption at 77 K and thermogravimetric analysis. The adsorption capacities of modified montmorillonite nanomaterials to remove Methyl Orange (MO) from aqueous solutions were studied as a function of contact time, solution pH, adsorbent dosage, initial MO concentration and temperature. The maximum removal efficiency of MO was found in acidic medium, with 60 min equilibrium time and 1 g/L adsorbent dosage. The adsorption kinetics and isotherms were well fitted by pseudo-second order and Langmuir models. The montmorillonites intercalated with both cetyltrimethylammonium bromide and hydroxy aluminum polycation showed a high affinity for MO molecules. Moreover, thermodynamic results indicated an exothermic, a spontaneous and a physical adsorption process. The characterization and adsorption performance of cetyltrimethylammonium bromide intercalated montmorillonite (CTAB-Mt) and cetyltrimethylammonium bromide and hydroxy aluminum polycation intercalated montmorillonite (CTAB-Al-Mt) toward MO was also compared with that of the hydroxyl- aluminum pillared montmorillonite and purified montmorillonite (OH-Al-Mt).

Keywords: Methyl Orange, montmorillonite, adsorption, waste water, dyes.

EFFICIENT SYNERGY OF PHOTOCATALYSIS OF INDUSTRIAL TEXTILE OVER FERRIC DIATOMITE MODIFIED HYBRID PHOTOCATALYST UNDER VISIBLE-LIGHT IRRADIATION

Walid REZIG[*,1] **& Mohammed HADJEL**[2]

[1] *Laboratory of Sciences, Technology and Process Engineering ; Department of Chemical Engineering ; Faculty of Chemistry; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran; Oran; Algeria.*

[2] *Laboratory of Sciences, Technology and Process Engineering; Department of Physical Chemistry; Faculty of Chemistry; University of Sciences and the Technology of Oran Mohamed Boudiaf USTO-MB ; BP 1505 El M'naoueur Bir El Djir 31000 Oran; Algeria.*

Corresponding Author: walidrzg@gmail.com

Abstract

Silica coated hematite nanoparticles "SCHN" composite as catalyst and characterized in this study. SCHN was made a surface modification treatments including Iron (III) nitrate nanohydrate $Fe(NO_3)_3.9H_2O$ deposition on raw diatomite .In the $Fe(NO_3)_3.9H_2O$ treatment, surface silica of diatomite and TiO_2 degussa P25 were partially dissolved in The iron (III) nitrate nanohydrate $Fe(NO_3)_3.9H_2O$ by means of x-ray fluorescence (XRF), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and UV-visible diffuse reflectance spectroscopy (DRS).The surface area of SCHN is 855 m^2/g. The surface modification also increased the point of zero charge (pH_{PZC}) values to 6 for Silica coated hematite nanoparticles with gap band was Eg=1.1 eV by UV-visible DRS technique. The colour removal of vat green 03 indanthren in different pH's using the diatomite modified TDF. It was observed that the vat green 03 indanthren textile dye degradation has pH dependency, the better result is at pH = 10.

Keywords: Silica, hematite, nanoparticles, Iron, gap band.

ZEOLITE OMEGA, AN ENVIRONMENTALLY-FRIENDLYCATALYST FOR THE SYNTHESIS OF CYCLIC ENAMINES

Ferial KORICHI*, Nabila BOUCHIBA, Hamza BENAOUDA

Department of Department of exact and applied sciences, Faculty of chemistry, UniversityOran1 Ahmed Ben Bella, El-Mnaouer, BP 1524, 31000, Oran, Algeria
Corresponding Author: Korichiferial@outlook.com

Abstract

Zeolite omega was successfully synthesized using both the direct crystallization method and the germination method, which separates the nucleation and crystal growth stages.

The performance of zeolite omega as a catalyst was evaluated in the synthesis of cyclic enamines. The synthesized samples were subjected to various characterization techniques, including XRD, nitrogen sorption at 77 K, FTIR, TGA, NMR and SEM.

The results showed that the designed omega zeolite crystals exhibited distinct morphologies and textural properties .Furthermore, the use of the germination method enabled the formation of zeolite omega with lower amounts of template compared to the direct crystallization method.

Catalytic evaluation revealed that zeolite omega samples, after proton exchange, achieved remarkable enamine yields (97%) and significantly reduced reaction times compared to conventional catalysts.

The stability of the H-omega catalyst was confirmed, as it retained its activity over fiveconsecutive experiments without any noticeable decrease

Keywords: zeolite omega, synthesis, characterization, germination method, catalyst

NEW METHOD FOR NUCLEOPHILIC SUBSTITUTION ON HEXACHLOROCYCLOTRIPHOSPHAZENE BY DIETHANOL AMINE USING AN ALGERIAN PROTONEXCHANGED MONTMORILLONITE CLAY (MAGHNITE-H^+) AS A GREEN SOLID CATALYST

Lahouaria MEDJDOUB*[,1] & Souad BENNABI[2]

[1]*Department of Preparatory classes, Higher School of Biological Sciences of Oran (ESSBO), 31000, Oran, Algeria*
[2]*Department of Chemistry, Faculty of Exact Sciences and Informatics, University of Hassiba Benbouali, B.P 78C, Ouled Fares, Chlef, Algeria*
Corresponding Author: houariamejdoub@yahoo.fr

Abstract

Nucleophilic substitution on hexachlorocyclotriphosphazene (HCCTP) with diethanolamine in order to give hexa(diéthanolamino)cyclotriphosphazene (HDCTP) is performed for the first time under mild conditions by using diethylether as solvent to replace benzene which is very toxic.The reaction time is reduced to half and also performed at room temperature but especially in the presence of an eco-catalyst called Maghnite-H^+. This catalyst has a significant role in the industrial scale. In fact, the use of Maghnite is preferred for its many advantages: a very low purchase price compared to other catalysts, the easy removal of the reaction mixture. Then, Maghnite-H^+ is became an excellent catalyst for many chemical reactions. The structure of HDCTP synthesized in the presence of Maghnite-H^+ to 5% by weight is confirmed by ^{1}H-NMR, ^{13}C-NMR, ^{31}P-NMR (Nuclear magnetic resonance) and FTIR (Fourier Transform Infrared spectroscopy). MALDI-TOF (Matrix-Assisted Laser Desorption/Ionisation-time-of-flight mass spectrometry) is used to establish the molecular weight of HDCTP which is 471 g/mol. DSC (Differential Scanning Calorimetery) and TGA (Thermogravimetric Analysis) show that HDCTP is a crystalline product with a melting point of 88°C. It is reactive after melting but is degraded from 230°C. In this work, a new synthetic method was developed to produce HDCTP using friendly, green, ecologic and non toxic catalyst clay as proton source avoiding the use of benzene as asolvent because it is carcinogenic, so it is re-placed by diethyl ether which is less toxic. The synthesis of HDCTP is also carried out at room temperature with a halving of reaction time from 24 to 12 h which is very attractive from an industrial point of view.

Keywords: Hexachlorocyclotriphosphazene, Diethanolamine, Organophosphazene, Maghnite- H^+, MALDI-TOF, RMN.

DEGRADATION D’UN POLLUANT ORGANIQUE EN UTILISANT DES DERIVES D’ORTHOFERRITES A BASE DE LANTHANE

Achouak ACHOUR[*,1], Necira ZELIKHA[2], Abba MALIKA[1], Rahal RAHIMA[1]

[1] *Laboratoire de chimie moléculaire et environnement(LCME), faculté des Sciences Exactes et dela Vie .Biskra*
[2] *Laboratoire de chimie appliquée(LCA), faculté des Sciences Exactes et de la Vie .Biskra*
Corresponding Author: achouak.achour@univ-biskra.dz

Résume

L’intérêt pour les matériaux pérovskites n’est pas nouveau, car ceux-ci, de structure Générale ABO_3, ont des propriétés très spécifiques selon les éléments cationiques A et B, que l’on peut choisir dans une large gamme d’éléments du tableau périodique. Citons des propriétés de piézoélectricité, de multiferroisme, de thermoélectricité, …. Les pérovskites à base de Terres Rares (éléments regroupant les quinze Lanthanides, l’Yttrium et le Scandium) et de métauxde transition ont fait l’objet de nombreux travaux.

L’objectif de ce travail est d’étudier des matériaux similaires, qui a des excellentes propriétés structurels et au même temps photocatalytiques. Pour cela, nous sommes partis de pérovskites de Terres Rares à base de fer et lanthane de formule générale lanthane $LaFeO_3$.

A notre travail ont porté sur la substitution cationique et anionique du composé $LaFeO_3$, élaboré par la méthode classique (synthèse par voie solide), et les produits obtenues sont caractérisées (caractérisations optiques, électriques et structurales) par BET, DRX, FTIR, MEB et UV-Vis , pour voir l'influence de la substitution sur les propriétés de notre produit de base qui est le $LaFeO_3$.

Mots clés : Pérovskite, photocatalyse, terre rare, dopage.

APPLICATION OF MESOPOROUS MATERIALS CATALYST IN ORGANIC REACTION

Nadia BOUGHEDIR[*,1,2] **& Zohra BAILICHE**[1,2]

[1] *Laboratory of catalysis and synthesis in organic chemistry, University of Tlemcen, BP 119, 13000, Tlemcen, Algeria.*
[2] *Science Institute, University of Ain Temouchent, BP 284, 46000, Ain Temouchent, Algeria*
Corresponding Author: boughedirnadia95@gmail.com

Abstract

This masters Works is divided into two parts :

The first part is a contribution to the study of mesoporous materials presenting a potential mainly in the field of catalysis. Ag/SBA15 mesoporous materials were synthesized under acidic conditionusing the copolymer triblock (pluronic123) as template and tetraethoxysilane (TEOS) as the source of silica. Heteroatoms such as silver have been incorporated by the post-synthesis pathway within the porosity of mesoporous materials to modify the latter of hexagonal structure and specific surface area. POWDER XRD, N_2 adsorption, FTIR Fourier transform Infrared techniques were used for characterization of catalysts and study of relationships with catalytic activity

The second part concerns the application of catalysts in the esterification of fatty acids we studied the influence of reaction parameters on the activity and selectivity of prepared catalysts and their applications in the production of biodiesel , for their many environmental and economic benefits. Biodiesel is a product obtained by esterification in which the fatty acid is reacted with an alcohol in the presence of a mesoporous catalyst. The esterification process is influenced by the reaction mode the molar ratio of the alcohol to the fatty acida , the type of alcohol, the nature and amount of the catalysts ,the reaction time, the content of the reaction metal, and temperature.

Keyword: Mesoporous, SBA15, Ag, post-synthesis, fatty acid esterification, methyl ester, biofuel biodiesel.

PREPARATION AND CHARACTERIZATION OF GRAPHENE NANOSHEETS (GNS)FROM GRAPHITE TAILINGSRECOVERED FROM DRILLING MOLD)

K. HADJ DJILANI, M. MAKHLOUF, S. BOURICHE, M. KADARI

[1] *Department of Faculty of Exact and Applied Science., Faculty of chemistry, University oran1,Postal code 31000, Oran, Algeria,*
[2] *Laboratory for the study of science and the environment and materials Oran1 -Algeria*
[3] *Laboratory of Energy Processes and Nanotechnology LPEN (EX FUNDPAL) university of Blida-Algeria*
[4]*Combustion, detonation and ballistics research laboratory .AMCDPHB Tipaza-Algeria*
Corresponding Author: sigma.hadj1983@gmail.com

Abstract

Graphite is a stack of carbon layers where carbon atoms from hexagons in a honeycomb structure graphene on the other hand is a single atom thick layer which offers unique physical chemical and biological properties compared to graphite Recycling graphite waste and converting it into graphene may offer many economic, environmental and health benefits and may also be used in many applications. Graphite has been used widely in iron-steel, chemical, and nuclear industries for electrical mechanical and other applications (e.g., metallurgy, pencil, coatings, lubricants and paint); and especially, most of the mold materials of drilling are madeof graphite.

The major goal of this study is to produce recycled graphene from graphite waste recovered from the drilling mold by using Hummer's method.

In this study, graphite-based tailings recovered from drilling mold were collected from local waste collection companies after the sieving and cleaning processes, the resulting graphite is exfoliated in a single layer using a chemical exfoliation. We herein present a simple, fast, efficient and environmentally friendly technique to prepare graphene (G) from graphite residues recovered from the drilling mold by using Hummer's method

Complete characterization of the properties of GO films have been performed. SEM and Raman analyzes showed that the G sheets prepared in this study had a double-layered and multilamellar structure-ray diffraction (XRD) was chosen to measure the crystal structure of our materials. A Fourier transform infrared (FT-IR) spectrum analyzer was used to certify the presence of oxygen-containing functional groups in G films. The chemical structure of the G sheet was described in this study. Discussion and references for further research on grapheneare provided.

Keywords: Graphene, Graphite, recycled, characterization

DEVELOPMENT AND CHARACTERIZATION OF A CATALYST BASED ON A METAL SUPPORTED ON PLANT MATERIAL FOR THE ELIMINATION OF ORGANIC POLLUTANTS IN THE LIQUID PHASE

Ghania HENINI[*,1], Ykhlef LAIDANI[1], Salah HANINI[2]

[1]Laboratory Environment-Water, Chlef University, P.O. Box 151, Hay Essalem, 02000 Chlef, Algeria
[2]Laboratory Chemical Plant - Water – Energy, Chlef University, P.O. Box 151, Hay Essalem, 02000 Chlef, Algeria
[3]Medea University, LBMPT, Urban Pole, 26000 Medea, Algeria
Corresponding Author: g.henini@gmail.com

Abstract

Discharges from the textile industry constitute enormous nuisances for human health and the environment. In fact, the various dyes used cause serious problems due to their stability and low biodegradability. Thus, it is necessary to treat these discharges before they are discharged into the sewerage network. The treatment of colored water has been the subject of several studies in order to reduce the intensity of the color and the organic matter contained in these waters.

Among the methods proposed are: coagulation, ultrafiltration, reverse osmosis, adsorption on activated carbon and biological treatments. Unfortunately, they are expensive, which has encouraged the search for other competing methods.

In this work, we have developed a catalyst based on a metal supported on a local plant material for the elimination of industrial organic pollutants. The product obtained will be characterized by different methods. A kinetic study will be carried out in order to study the effect of nanoparticle catalyst as well as the contact time on this catalyst. The Methylene Blue elimination rate decreaseswith increasing initial concentration.

Keywords: Industrial organic pollutant, Agricultural residues, Adsorption, XRD, FTIR, UV

THE PHOTOCATALYTIC EFFICIENCY OF A NATURAL MATERIAL IN THE DEGRADATION OF A DYE

Ykhlef LAIDANI[1], Ghania HENINI[1], Salah HANINI[2]

[1]Laboratory Environment-Water, Chlef University, P.O. Box 151, Hay Essalem, 02000 Chlef, Algeria
[2]Laboratory Chemical Plant - Water – Energy, Chlef University, P.O. Box 151, Hay Essalem, 02000 Chlef, Algeria
[3]Medea University, LBMPT, Urban Pole, 26000 Medea, Algeria
Corresponding Author: l.ykhlefi@gmail.com

Abstract

Various processes for processing textile dyes have been developed: physical, chemical, and even biological processes, and current trends should aim at integrating various technologies to process dyes at low cost. The different types of dye treatment studied so far solve only part of the problem. Indeed, most of the proposed methods remain insufficient and incomplete or even limited. Adsorption by activated carbon is among the processes used for the treatment of dyes with success, but its cost remains very high especially for underdeveloped countries. Similarly, advanced oxidation by the Fenton process has been the subject of several studies to eliminate textile dyes. In this work, we studied the removal of synthetic dye by adsorption and photocatalysis. This study allowed us to evaluate the influence of certain parameters: pH, adsorption capacity, effect of initial concentration, effect of mass, dye adsorption isotherms and adsorption kinetics for different systems. During this study, we also showed the effectiveness of the coupling for different parameters, namely: pH effect, effect of the initial concentration.

Keywords: Industrial organic dye, TiO_2, Industrial organic pollutant, Adsorption, Photocatalysis

PREPARATION AND CHARACTERIZATION OF POLY(GMA)@ RU/TIO_2@FE_3O_4 NANOCOMPOSITES FOR PHOTOCATALYTIC REDUCTION OF ORGANICPOLLUTANTS.

Mohammed Aymen ZORGANI*[,1], Farouk ZAOUI [1,2], Fatima Zohra SEBBA[1] , Roquiya nour el houda ZORGANI[1]

[1]Laboratoire de Chimie Physique Macromoléculaire L.C.P.M, Université Oran1 Ahmed BenBella, El-Menaouer, B.P 1524, 31000 Oran, Algérie
[2] Centre Universitaire El Cherif Bouchoucha -Aflou-, B.P 306, Aflou, Laghouat, Algérie
Corresponding Author: aymenzorgani98@gmail.com

Abstract

This work concerns the preparation of a new composite material based on poly(Glycidyl methacrylate), Ru/TiO_2 and Fe_3O_4 using ultrasound treatment. Several composites were prepared by varying the percentage of Ru/TiO_2 and Fe_3O_4. Then, they were applied as catalysts for the reduction of several organic pollutants. 4-Nitrophenol (4-NPh), Methylene blue (MB) and Orange G (OG) were used as a model to study the photocatalytic reduction process in the presence of $NaBH_4$ at room temperature. The obtained photocatalysts were characterized by different methods such as XRD, FTIR, SEM, TEM, TGA, ultraviolet–visible (UV–vis) spectroscopy. The results showed that the use of ultrasound gave a good dispersion of all species into the polymeric matrix. These solids have shown good activity via the photocatalytic reduction of organic pollutants. The best performance was obtained for the photocatalyst having the higher content of metal NPs “CP(30)”. The rate constant Kapp of composite CP(30) towards catalytic reduction of MB, OG and 4-NPh reached a high level up to 0.55 min^{-1}, 0.241 min^{-1} and 0.3 min^{-1}, respectively. Finally, the recyclability of the photocatalyst CP(30) was also evaluated. The results showed that the performance of this photocatalyst was satisfactory during its reuse.[1,2]

Keywords: Poly(Glycidyl methacrylate), RuNPs,TiO_2, Fe_3O_4, Ultrasound treatment, Catalysts, Reduction

UTILISATION DES DECHETS AGRICOLES POUR LETRAITEMENT DES EAUX

Nawel ZERROUKI* & Ahmed BOUCHERDOUD

Université de Relizane, Faculté des sciences et technologie, Département de chimie, 48000 Relizane, Algérie
Corresponding Author: zerroukin48@gmail.com

Abstract

La question de l’eau, problématique récurrente, est l’une des plus stratégiques de notre temps et des plus difficiles parce qu’elle est associée à la vie et qu’elle n’est pas le produit de l’homme. Dece fait, la pollution des eaux, accidentellement ou volontairement, devient un fléau universel qui entraîne la dégradation de l’environnement,

Comme tous les polluants nocifs, les effluents colorés nécessitent un traitement approprié avant de les déverser dans la nature. Pour cela, divers procédés de traitement sont appliqués. Parmi les procèdes de traitement des rejets liquides, l’adsorption reste une technique relativement utilisée et facile à mettre en œuvre. La recherche d’un adsorbant efficace et moins couteux s’avère intéressante.

Cette étude s’inclus dans ce cadre environnementale et économique et vise d’utiliser des adsorbants naturels abondants dans la nature à faible cout destinées aux traitements des rejets liquides chargées en effluents colorés et toxiques.

Ce travail consiste à étudier l’élimination de colorants à partir des solutions aqueuses par adsorption sur un biosorbant cellulosique abondant les feuilles de raisin laver et sécher qui peut concurrencer les matériaux classiques

Une étude cinétique d’adsorption par le test de l’influence de divers condition opératoire telles que : l’effet du temps de contact l’effet de la masse et du pH de la solution aqueuse. Cette cinétique a été modulée par plusieurs modèles mathématiques à savoir l’équation du pseudo- premier/deuxième ordre. Les isothermes de l’adsorption ont été établies par des tests de l’influence de la concentration sur la qualité du colorant adsorbée en appliquant les différents modèles (Langmuir, Freundlich et Temkin) et une étude thermodynamique a été examinée par la modification de la température du milieu réactionnel.
Malgré l’emploi du biosorbant brut sans prétraitement préalable et une faible surface spécifique mais riche en sites actifs les résultats obtenus ont montré que l’exploitation des résidus et des déchets banales non toxiques peut servir l’environnement et l’économie au même temps.

Keywords: Environnement, pollution, colorants, biosorbant, adsorption.

UTILIZATION OF NIO FOR MONTMORILLONITEMODIFICATION: APPLICATION FOR METHYLENE BLUE ADSORPTION

Horiya BOUKHATEM*, Sara SELAMI & Selma ZERAIF

Department of Mater Sciences, Faculty of Sciences and Technology, University DjilaliBounaama of Khemis-Miliana, 44225, Khemis-Miliana, Algeria
Corresponding Author: boukhatem_houria@yahoo.fr

Abstract

The discharge of dyes wastewaters directly into rivers and lakes even at very lowconcentrations can endanger living organism and its aquatic ecology because of their toxicity due to the aromatic structures. The treatment of dyeing wastewater is a great topic of research and one of the difficult challenges. Among all the treatment processes, adsorption has been proven more attractive and effective due to higher efficiency, lower cost, simplicity of operation and lower sensitivity to toxic pollutants.

In this study, the adsorptive removal of Methylene Blue (MB) from aqueous solutions onto nickel oxide modified montmorillonite (NiO-Mt) and commercial bentonite has been studied. The influence of some experimental factors such as contact time, initial dye concentration and temperature was investigated. Batch adsorption studies manifested that the maximum adsorption capacity of MB was around 99.9 mg/g in 10 min at initial concentration of 100 mg/L and ambiant temperature of 25°C. The adsorption isotherms were well fitted by Langmuir model and the adsorption kinetics were better by pseudo-second-order model. The thermodynamic parameters such as the changes in Gibbs free energy (ΔG°), enthalpy (ΔH°), and entropy (ΔS°) were determined. The MB adsorption was physical, spontaneous and exothermic for both adsorbents.

Keywords: NiO-Mt, commercial bentonite, Methylene blue, Adsorption.

CALCIUM ALGINATE ENTRAPPED DATE PITS POWDERFOR CATIONIC DYE ADSORPTION FROM AQUEOUS SOLUTION: EXPERIMENTAL, OPTIMIZATION AND DFT STUDY

Soumia ABDELKRIM*,[1], Adel MOKHTAR[1,2], Amina SARDI[3], Bouhadjar BOUKOUSSA[1]

[1] Laboratory of Materials Chemistry L.C.M, University Oran1 Ahmed Ben Bella, BP 1524, El-Mnaouer, 31000 Oran, Algeria
[2] Department of Process Engineering, Faculty of Science and Technology, University of Relizane,48000 Relizane, Algeria
[3] Department of Chemistry, Faculty of Exact Sciences and Computer Science, University ofHassiba Ben Bouali, Chlef, 02000, Algeria
Corresponding Author: abdelkrim_soumia@yahoo.fr

Abstract

Biodegradable and very low-cost adsorbent beads were prepared from date pits powder (DP) and sodium alginate (SA). DP to SA ratios was varied (1/2, 1/4 and 1/6) and used to eliminate Crystal violet (CV) a cationic dye. Adsorbents were characterized by FTIR, SEM-EDS, UV-vis DR, TGA and the point of zero charge (pH_{PZC}). The optimal composite beads SA@6DP show high adsorption capacities of 83.565 mg/g toward CV than SA@2DP and SA@4DP. The kinetics investigation showed that the adsorption is well described by the pseudo-second-order kinetic (R^2 =0.998). The thermodynamics and isotherms studies exhibit that the adsorption phenomenon for SA@6DP adsorbent is endothermic and significantly fitted with the Redlich- Peterson model. The experimental adsorption tests were optimized by the Box-Behnken design (BBD) which led to conclude the maximal CV removal obtained by SA@6DP was 99.873% using [CV]= 50 mg/L, adsorbent mass= 20 mg and 48 h of contact time. The theoretical calculation proved that the CV molecules favor the mode of attack due to their electrophilic character and can accept the SA@6DP adsorbent electrons more easily to form an anti-bonding orbital. SA@6DP hydrogel beads are therefore an exceptional bio-adsorbent that offers excellent adsorption performance.

Keywords: Sodium alginate, Crystal violet, Adsorption, Optimization, DFT study.

SYNTHESIS, CHARCATERISATION AND APPLICATION OF NEW BIOCOMPOSITES

Amel MEKKI *[1,2], Bouhadjar BOUKOUSSA [1,3], Mohammed HACHEMAOUI [1,3], Adel MOKHTAR[1,3]

[1] *Laboratoire de Chimie des Matériaux L.C.M, Université Oran1 Ahmed Ben Bella, BP 1524, El-Mnaouer, 31000 Oran, Algérie*

[2] *Ecole supérieure en sciences biologiques d'Oran ESSBO BP1042 Saim Mohamed, cite Emir Abdelkader Ex INESSMO, Oran Algérie*

[3] *Département Génie des Procédés, Institut des Sciences et Technologies, Université Ahmed Zabana, 4800 Relizane, Algérie*

Corresponding Author: mekki.amel3@gmail.com

Abstract

This work concerns the preparation of a new composite based on alginate and zeolite omega modified by different nanoparticles (MNPs: Co, Cu and Fe). Firstly, the calcined zeolite omega was exchanged by different divalent metals and in the second step was encapsulated by calcium alginate to obtain a composite in the form of beads. The latter were chemically treated with a reducing agent $NaBH_4$ to transform the metal cations into nanoparticles. Several techniques such as XRD, XRF, FTIR, XPS, SEM and TGA were used to characterize the obtained samples.

The different samples were tested via two different applications. The first consists on the catalytic reduction of the MB dye under $NaBH_4$, several parameters affecting this reaction have been investigated and discussed. The second application consists on the use of these samples as antibacterial and antifungal agents via different strains.

The obtained results showed that all the samples were effective towards the reduction of MB dye. The composite Co/Zeolite@ALG was selected as the best performing catalyst due to its reduction of MB dye being completely achieved in 3 min with a rate constant of 1.4 min^{-1}, which was attributed to its highly porous structure. The results of the reuse of the best catalyst showed that this catalytic system was stable for five successive cycles without losing its catalytic properties.

Keywords: Composites beads, Catalytic reduction of MB dye, nanoparticles, zeolite, omega

SYNTHESIS OF BIOMASS-DERIVED ACTIVATED CARBONS AND THEIR IMMOBILIZATION ON ALGINATE GELS FORTHE CATALYTIC REDUCTION OF AZO DYE

Fatma CHERGUI*[,1], Adel MOKHTAR[1,2], Soumia ABDELKRIM[1], Boubekeur ASLI[2], Mohamed SASSI[1]

[1] *Laboratory of Materials Chemistry L.C.M, University Oran1 Ahmed Ben Bella, BP 1524, El- Mnaouer, 31000 Oran, Algeria*

[2]*Department of Process Engineering, Faculty of Science and Technology, University of Relizane,48000 Relizane, Algeria*

Corresponding Author: fach1743@gmail.com

Abstract

Nickel oxide nanoparticles supported activated carbon (AC-NiO) was fabricated using thermal activation. Then, AC-NiO composite was immobilized on alginate beads to obtain 3-dimensional network structure ALG@AC-NiO nanocomposite beads for catalytic reduction of Congo red (CR) dye. The resulting nanocomposite beads were identified by various physical techniques. The crystalline nature and dispersion of NiO nanoparticles was defined by the XRD and EDS techniques, respectively. ALG@AC-NiO beads have a Ni element content of 4.65wt% with an average NiO particle diameter of 23 nm. The statistical approach mathematically describes the catalytic reduction of the CR dye as a function of the $NaBH_4$ concentration, the catalyst dose and the concentration of the CR dye modeled by a BBD-RSM. According to the statistical modeling and the optimization process, the catalytic optimum conditions were obtained for $NaBH_4$ concentration of 0.05 M, catalyst dose of 11 mg and CR dye concentration of 80 ppm who permit meet 99.67% of CR dye conversion. The adjusted coefficient of determination ($R^2 = 0.9957$) indicates that the considered model was quite suitable with a good correlation between the experiment and predicted.

Keywords: Sodium alginate, Activated carbon, NiO, Composite beads, Dye reduction.

KINETICS AND THERMODYNAMIC STUDIES FOR REMOVAL OF TRYPAN BLUEAND METHYLENE BLUE FROM WATER USING NANO CLAY FILLED COMPOSITE OF HTAB ANDPEG AND ITS ANTIBACTERIAL ACTIVITY.

Amina SARDI*[,1,2], Souad BENNABI[2], KRADRA BRAHMA Khadidja[1,2], Boumediene BOUNACEUR[1], ABDELKRIM Soumia[3,4],Adel MOKHTAR[5,4], Bouhadjar BOUKOUSSA[4,6], Miloud TAHAR ABBES[7,8],

[1] Laboratoire de Chimie Physique Macromoléculaire L.C.P.M, Université Oran 1 Ahmed BenBella, El-Menaouer, B.P 1524, 31000, Oran, Algérie
[2] Université Hassiba Ben Bouali, Faculté science exacte et informatique, département de chimie,02010, Ouled Fares, Chlef
[3] Département de Chimie, faculté des sciences exactes et appliquées, Université Oran 1 AhmedBen Bella, El-Menaouer, B.P 1524, 31000, Oran, Algérie
[4] Laboratoire de Chimie des Matériaux L.C.M, Université Oran1 Ahmed Ben Bella, BP 1524, ElMnaouer, 31000 Oran, Algérie
[5]Département Génie des Procédés, Faculté des Sciences et Technologies, Université de Relizane,48000 Relizane, Algérie
[6]Département de Génie des Matériaux, Faculté de Chimie, Université des Sciences et de laTechnologie Mohamed Boudiaf, BP 1505, El-Mnaouer, 31000 Oran, Algérie
[7]Laboratoire de mécanique et énergétique (LME), Faculté de technologie, Université Hassiba BenBouali Chlef, Hay Salem National Road No 19, 02000 Chlef, Algérie
[8]Département de Génie mécanique, Faculté de technologie, Université Hassiba Ben BoualiChlef, 02000 Chlef, Algérie
Corresponding Author: a.sardi@univ-chlef.dz

Abstract

In the submitted research study, the adsorption properties of Montmorillonite (MMT) modified with surfactant HTAB (MMT@HTAB) and then with polymer PEG (MMT@HTAB@PEG) for anionic trypan blue (TB) and cationic methylene blue (MB) dyes from aqueous media were explored. The prepared adsorbents were characterized by XRD, FTIR, SEM and zeta potential measurement. To study their adsorption capacities and the mechanisms for TB and MB adsorption, batch adsorption investigation were performed by adjusting the adsorbent/adsorbent contact time, pH medium, initial dye concentration and temperature effect. The maximum adsorption capacity of TB and MB was found to be 190.81 and 237.22 mg/g, respectively, with MMT@HTAB@PEG adsorbent in an initial concentration of 100 mg/L at alkaline pH in 35 min and a temperature of 25°C. The adsorption kinetics of TB and MB on MMT@HTAB@PEG was best fitted by the pseudo-second order model, indicating that the process is chemisorption. The Freundlich result reveals better consistency than the Langmuir model, indicating that the adsorption is favorable and in the form of multilayers. The thermodynamic study showed that the adsorption processes of TB and MB by the both MMT@HTAB and MMT@HTAB@PEG adsorbents occur in an autonomous way and the temperature has not a significant effect on the adsorption capacity of TB and MB dyes. In addition, MMT@HTAB showed good antibacterial activity against both Escherichia coli (ATCC 8739) and Micrococcus luteus (ATCC 9341) bacteria compared to MMT@HTAB@PEG. The broadcast area was found to be 6 and 5 mm in Escherichia coli (ATCC 8739) and Micrococcus luteus (ATCC 9341), respectively.

Keywords: Montmorillonite, PEG, Dyes, Hybrid composite, Adsorption.

EFFECTS OF DRY TIME ON THE OPTICAL PROPERTIES AND CATALYTIC APPLICATIONS OF NIO THIN LAYERS PREPARED BY DIP COATING PROCESS

Mohammed ATMA*,[1], Melia HAMICI[2], Khalifa HEDDADI[1]

[1] Department of Physics, Faculty of Science, University of Ferhat Abbas-Setif1, 19000, Setif,Algeria
[2] Department of basic education in technology department, Faculty of technology, University ofFerhat Abbas - Setif1, 19000, Setif, Algeria
Corresponding Author: mohammed.atma@univ-setif.dz

Abstract

In this work, we studied the impact of drying time on the optical properties and the catalytic potential of nickel oxide (NiO) thin films. NiO thin films were deposited on glass substrates by sol-gel immersion in a NiO precursor solution. for two different annealing temperatures (350 and 450°C) and different drying times (15, 25, 30 and 40 minutes), the thin layers were tested. UV-Visible spectroscopy was used to analyze the optical properties of these thin films, recording absorbance and transmission spectra in the wavelength range of 400–800 nm. The optical energy gap for direct electronic transitions was calculated using the Tauc equation. The results revealed that the band gap values ranged from 2.40 eV to 3.36 eV. the smaller gap is obtained for the layer drying for 40 minutes and an annealing temperature of 450°C. The catalytic efficiency varied between 16% and 28% after 2 hours of adsorption, depending on the mass of the catalyst used and the adsorption time. The optimal conditions were achieved by using the thin layer of NiO dried for 40 min annealed and annealed at 450°C 100 mg of catalyst. this layer gave the best methylene blue removal efficiency of 18%, in one hour of adsorption.

Keywords: NiO, dip coating route, dry time, optical energy gap, adsorption.

STUDY OF THE DEGRADATION KINETICS OF ORGANICDYES IN AQUEOUS SOLUTION BY PHOTOCHEMICAL DEGRADATION AND ADSORPTION ON ACTIVATED CARBON.

Bekhta MAIMOUN*,[1] & Lahcène DJAFER[2]

[1] Department of process engineering, Faculty of technology, University Hassiba Benbouali ofChlef, Postal code: 02000, City: Chlef, Country: Algeria.
[2]Hassiba Benbouali University, Water and Environment Laboratory
Corresponding Author: b_maimoun@hotmail.fr

Abstract

Industrial effluents from textile activities, tanneries, or printing companies often have a significant coloring pollutant load that is difficult to biodegrade. Their decontamination by techniques is in some cases ineffective. In this work, we investigated two distinct processes for theremoval of two synthetic dyes (ETL and Indigo Carmine), model molecules of pollutants.

In the first part, we were interested in the study of the adsorption of two dyes on commercial activated carbon. A systematic study allowed us to assess the influence of certain parameters on the adsorption capacity of the two dyes. In a second part, we tested the removal of the non-adsorbed contaminant from the activated carbon tip by the photocatalytic reaction using a TiO_2catalyst.The time required for absorption is 15 min for the two dyes with a maximum retention capacity, Q_e, equal to 4.7 mg/g for Bemacid red ETL and 6.82 mg/g for Indigo Carmine. The kinetics are controlled by pseudo-second order (R^2=0.985 and R^2=0.999).The Freundlich model describes the adsorption of ETL and Indigo Carmine dyes on activated carbon.

Experimental results have shown that the photocatalytic reaction gives good retention at low concentrations of dye solutions and that the rate of degradation increases with increasing initial dye concentration.

We were able to conclude that the coupling between the two processes (adsorption and photocatalysis on TiO_2) is effective for the treatment of colored water under experimental conditions.

Keywords: Adsorption, activated carbon, ETL, Indigo Carmine, photocatalytic.

REMOVAL OF PHOSPHATES FROM THE GL3/Z COMPLEX WWTP BYADSORPTION USING MAGHNIA BENTONITE

Ahlem Nacera KHELF* & Ghenia BENTABED ABABSA

Department of Chemistry, Faculty of exact and applied sciences, University Oran 1, 31000,Oran, Algeria,
Corresponding Author: ahlem_81@hotmail.com

Abstract

The aim of this work is to test the capacity and efficiency of bentonite in the GL3Z laboratory for the adsorption of phosphates present in liquid effluents from the natural gas liquefaction industry. Before starting the bentonite phosphate adsorption process, we carried out a phosphate analysis todetermine the exact value of phosphate in our sample. We then helped find the optimum operating conditions for the right material, its optimal quantity and the right pH of the medium.

The tests will be carried out by adsorption on bentonite in its raw state, thermally and chemically treated under mild operating conditions: at ambient temperatures and under atmospheric pressure. Mathematical modelling of adsorption isotherms has shown that the Freundlich model is more suitable than the Langmuir model, confirming that adsorption takes place in multilayers and at sites with different energies.

From the results obtained we can affirm that bentonite used as an adsorbent is effective for phosphate removal.

The natural abundance of this material and low investment costs could offer a good alternative to other more expensive adsorbents such as activated carbon or zeolites.

Keywords: Phosphate, adsorption, bentonite.

DEVELOPMENT OF BATIO3ZNO NANOCOMPOSITES MODIFIED BY A CUDOPANT FOR APPLICATIONS IN PHOTOCATALYTIC DEGRADATION OF AN ORANGE G DYE

Khadidja ESSELAMI[1], Khaled El MILOUDI[2], Sihem HENNAOUI[2], Mohammed SADOU[*,2], Mohammed HADJ MILIANI[2], Mouna AMARA[2]

[1]Department of chemistry, Faculty of Exact Sciences and Informatics, University Hassiba Benbouali, 21000, Chlef, Algeria,1
[2]LPTPM, Faculty of Technology, Hassiba Benbouali University of Chlef, 02000 Chlef, Algeria.
Corresponding Author: m.sadou@univ-chlef.dz

Abstract

The elimination of organic pollutants and in particular azo dyes which constitute one of the most important groups of pollutants released into wastewater by the textile industry and other industrial processes. These processes remain incapable of eliminating molecules recalcitrant organics. Various conventional treatment methods: physical, chemical and biological are widely used. New effluent treatment processes have established themselves thanks to their high cleaning power. Among these treatments, we cite advanced oxidation processes (POA) whichare attracting more and more attention as an alternative to treatment processes. Traditional. POAs are based on the in situ generation of highly oxidizing radicals, mainly hydroxyl radicals (HO●). A solid solution Cu $Ba_{0.4}Zn_{0.6}TiO_3$ was synthesized by the sol-gel method. An analysis carried out by (XRD) indicates the existence of a solid solution (mixed oxide) where Zinc completely replaces Copper; followed by an IR analysis reports all the vibrations characteristic of a mixed oxide compound. The results of UV-Visible spectroscopy showed that the compound Cu $Ba_{0.4}Zn_{0.6}TiO_3$ behaves as a good catalyst since the oxidation rate reaches almost 80%. As well as the oxidation results of a volume of 100 ml of the OG dye with a concentration of 25 mg/l while varying the parameters, show that advanced oxidation of Orange G dye is accessible for 0.025 g of Cu $Ba_{0.4}Zn_{0.6}TiO_3$ in the presence of 0.1 ml of H_2O_2. The kinetic studyof decolorization of Orange G dye shows that the pseudo first order model is the most reliable for determining the order of the oxidation kinetics of the ORG on the catalyst.

Keywords: Nanocomposites, dye, organic pollutants.

INFLUENCE OF HEAT-TREATED AND ACID-LEACHED ON HYDROPHOBIC CHARACTER AND ADSORPTION PROCESS OF MICROPOLLUTANT ON MODIFIED CLAY

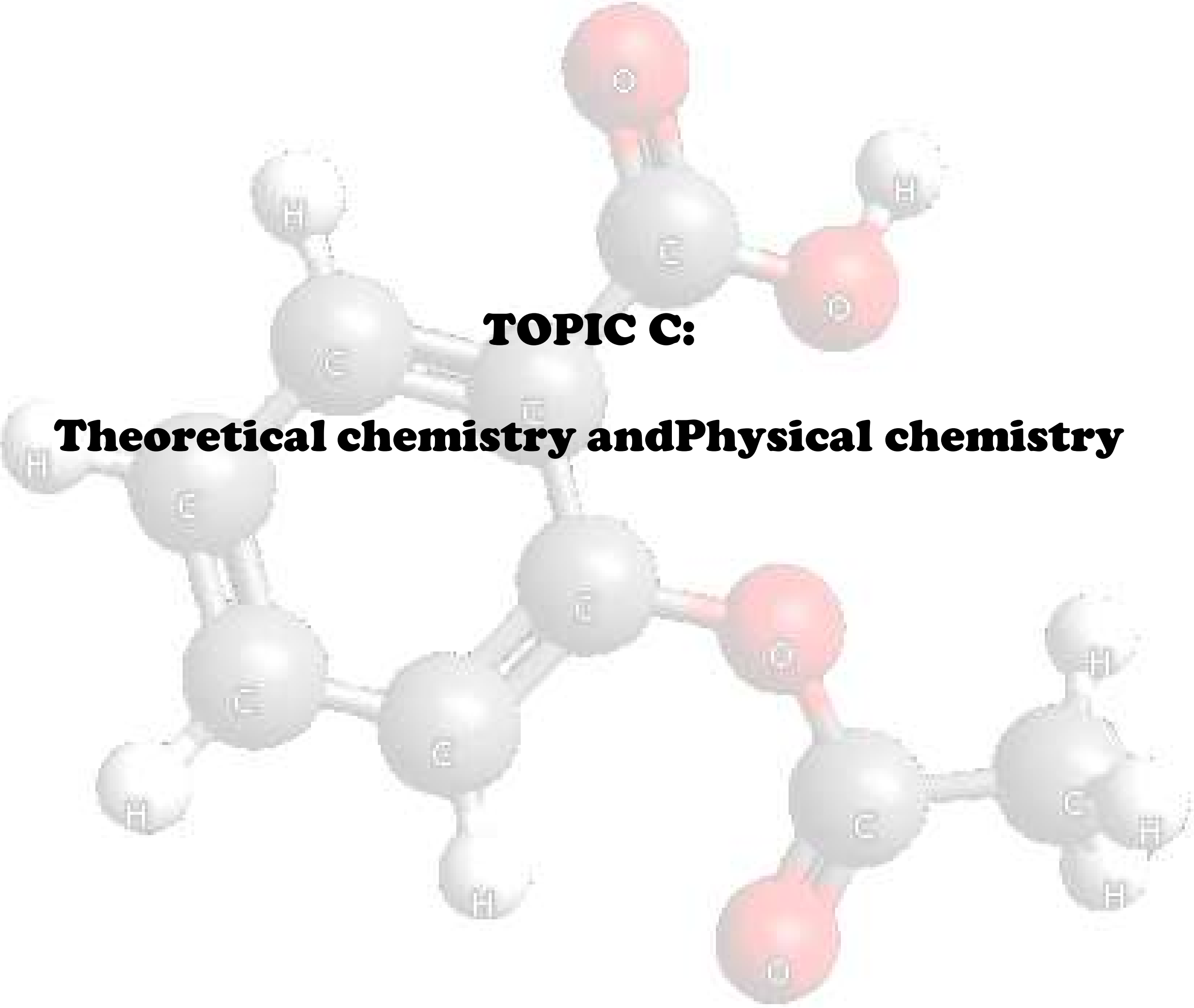
K. BELKASSA*[,1,4], M. KHELIFA[1], K. Marouf-KHELIFA[2], I. BATONNEAU-GENER [3], A. KHELIFA [1]

[a] Laboratoire de Structure, Elaboration et Applications des Matériaux Moléculaires (S.E.A.2M.),Département de Chimie, Université de Mostaganem, B.P. 981, R.P., Mostaganem 27000, Algérie
[b] Laboratoire des Sciences et Techniques de l'Environnement et de la Valorisation (S.T.E.V.A.), Département de Chimie, Université de Mostaganem, Algérie
[c] Institut de Chimie des Milieux et Matériaux de Poitiers IC2MP – UMR 7285 CNRS- Universitéde Poitiers, 4 rue Michel Brunet, 86022 Poitiers,
[d] Laboratoire synthèse et catalyse, Université de Tiaret 14000, Algérie
Corresponding Author: belkassakheira@yahoo.fr

Abstract

The Algerian halloysite, is a raw material, local, abundant and low cost. A literature search has shown that clays of type 1: 1, the case of halloysite, once modified, can reveal interesting adsorptive properties [1,2]. The modification of Halloysite consists of a structural change and a dealumination through a heat treatment at 600°C where an acid attack at different concentrations. The resulting materials were employed as crystal violet (CV^+) adsorbents from aqueous solutions. Hence, the interest of monitoring the hydrohobicity index is necessary for these materials. Hydrophobicity is a function of a number of factors [3,4], it is proposed to follow this index after the modification. The thermo-chemical treatments preserve the tubular morphology, the specific surface area increased significantly from 60.5 to a maximum of 503 m^2/g. The CV^+adsorption onto the modified halloysites is rapid in the first 10 min. The adsorbed quantity decreased with increasing temperature. The overall mechanism of CV^+ adsorption process by modified halloysites follows pseudo-second-order kinetics with the contribution of the intraparticle diffusion. Chemical treatment increases the hydrophobic nature of these changed halloysites according to the hydrophobicity indices calculated which make these materials useful in recovery of pollutants in aqueous phase.

Keywords: Hallolysite, Modification, hydrophobicity, crystal violet.



TOPIC C:

Theoretical chemistry andPhysical chemistry

THEORETICAL STUDY OF A NEW CONDUCTIVE COPOLYMER BASED ON N-VINYLCARBAZOLE

Hasnia ABDELDJEBAR[1], Mohamed BOUGUETAIB[2], Rachid MEGHABAR[2]

[1]Scientific and Technical Research Center for Physical and Chemical Analysis (CRAPC), BP 384, Bou-Ismail, RP 42004, Tipasa, Algeria.

[2] Polymer Chemistry Laboratory, Faculty of Exact and Applied Sciences, Department of Chemistry, University Oran 1 Ahmed Ben Bella, BP 1524, El M'Naouer, Oran, Algeria.

Corresponding Author: abdeldjebar_hasnia@yahoo.com

Abstract

Over the past thirty years, semiconducting polymers have undergone considerable development in academic research. More recently, they have begun to attract growing interest in the industrial world. Their use as active materials in a wide range of optoelectronic devices offers a real alternative to more conventional semiconductors.

In this work, we present theoretical calculations for the structural, spectral, electronic, thermodynamic and reactivity studies of a new synthesized copolymer based on N-vinylcarbazole by a new synthesis technique adopted by the Polymer Chemistry Laboratory of the University Oran 1 Ahmed Ben Bella (Es-Senia). These calculations were carried out by applying quantum chemical methods, using the 9th version of the GAUSSIAN program. These calculated physico-chemical parameters using the B3LYP functional with the 6-311G (d,p) basis set, have enriched the database for this new copolymer, and explained the various phenomena observed by the experimenters, in particular those linked to the structure and reactivity of this material. The motivating results have prompted us to complete the theoretical work by estimating its semi conductor potential in order to improve the properties of this material and thus increase its potential for industrial applications, particularly as an active material in optoelectronic and other devices.

Keywords: Semiconductor, theoretical calculations, N-vinylcarbazole, Gaussian 09, industrial application.

CALCUL THEORIQUE DU FACTEUR DE MERITE PARL'APPROXIMATION GGA D'UN NOUVEAU DEMI HEUSLER XYZ

Anissa BESBES*, Ali AISSANI, Radouan DJELTI

Département Sciences et technologie, Faculté des Sciences et technologie, LaboratoireTechnologie et Propriétés des Solides, Université de Mostaganem, 27000 , Algérie

Corresponding Author: anisseb17@yahoo.fr / anissa.djelti@univ-mosta.dz

Abstract

La performance thermoélectrique des matériaux semi-conducteurs est décrite par le facteur de mérite (Zt) qui doit avoir une valeur au voisinage de l'unité afin de permettre à ce type de matériaux une récupération de la chaleur résiduelle qui par la suite sera utilisée pour améliorer l'efficacité énergétique de tout processus générateur de chaleur.

Dans le présent travail, nous nous sommes basés sur la théorie de la fonctionnelle de densité (DFT) et précisément la méthode des ondes planes augmentées linéarisées (FP-LAPW) et l'approximation du gradient généralisée (GGA) pour faire une investigation théorique des propriétés structurales et thermoélectriques d'un nouvel alliage type demi-Heusler ternaire XYZ . L'étude des propriétés structurales de cet alliage montre qu'il se cristallise dans la structure cubique avec le groupe d'espace F43m (216) et les propriétés électroniques révèle qu'il a un caractère semi conducteur car il présente une bande interdite de gap indirect tandis que les propriétés thermoélectriques qui ont été calculés par la théorie semi classique de Boltzmann mise en œuvre dans le code BoltzTraP, ont montré que ce matériau présente une conductivité électrique élevée et une faible conductivité thermique. Ces caractéristiques lui confèrent une valeur du coefficient ZT élevée dans une large plage de température, ce qui lui procure la possibilité d'être utilisé dans le domaine thermoélectrique.

Keywords: DFT, Demi Heusler, semi conducteur , propriétés thermoélectriques, facteur de mérite

AUTOMATED SAMPLE PREPARATION FOR MONOCLONAL ANTIBODIES FINGERPRINTING BY CAPILLRY ELECTROPHORESIS

Meriem DADOUCH*[1,2], Yoann LADNER[3], Claudia BICH[3], Jérome MONTELS[3], Jaques MOREL[4], Catherine PERRIN[3]

[1] *Department of pharmacy, Faculty of Medecine., University of Djilali Liabes, 22000, Sidi Bel Abbes, Algeria,*
[2] *Laboratory of Physical Chemistry of Macromolecules and biological interfaces, University of Mustapha Stambouli, 29000, Mascara, Algeria,*
[3] *UMR 5247-CNRS-UM-ENSCM, Institute of Biomolecules Max Mousseron (IBMM), University of Montpellier, 34293, Montpellier, France,*
[4] *Department of Rhumatology, Lapeyronie Hospital, 34295, Montpellier, France.*
Corresponding Author: dadouch.meriem@gmail.com.

Abstract

Capillary electrophoresis (CE) is a promising technique for automated sample preparation integrated with electrophoretic separation of reaction products. Here, the development of fast automated and integrated methodology for the routine quality control of monoclonal antibodies (mAbs) at the bottom-up level is described. First, simultaneous denaturation and reduction (pretreatment step) were conducted with RapiGest® surfactant and dithiothreitol. Then, in-line sample preparation was realized by transverse diffusion of laminar flow profile under controlled temperature. In-line digestion was carried out with an autolysis-resistant trypsin to generate digested mAb electrophoretic profiles free from trypsin peptides interferences. The main parameters affecting the digestion (trypsin concentration and incubation conditions) were optimized to get high digestion efficiency in short time. An acidic mass spectrometry-compatible background electrolyte was used to obtain high resolution separation of released peptides and in-line surfactant cleavage. The whole methodology was performed in less than two hours with good repeatability of migration times (RSD=0.91%, n=5) and corrected peak areas (RSD = 9.6%, n = 5). CE-fingerprints were successfully established for different mAbs and an antibody-drug conjugate.

Keywords: Capillary electrophoresis, monoclonal antibodies, trypsin, transverse diffusion of laminar flow profile, sample preparation.

SOME IDENTIFIED DIATOMIC MOLECULES PROPERTIES USING THEWKB APPROXIMATION

Khalid REGGAB

Department of Physics, Faculty of exact sciences and Informatics, University Ziane Achour ,17000, Djefla, Algeria,
Corresponding Author: khaledreggab@gmail.com

Abstract

The equation developed by Schrödinger for an arrangement of electrons that experiences both the attracting Electrostatic interaction from the center of the atom and the repulsion Electrostatic force among every pair of electrons has been a difficulty for quantum physicists. Chemical reactions are represented in quantum physics by the function of wave that contains all the details regarding the system's current state, and the Schrödinger equation determines how they act. Schrodinger equation can be solved in a variety of methods, in this study, we employed the WKB approach to take advantages of the perturbed harmonic potentialto tackle the problem of recognizing the energy-bound phases. Here, we present the WKB theory and construct the Schrödinger equation solutions based on the WKB approximation by determining the energy eigen values in the existence of the perturbed harmonic potential. We utilized the energy final formula that stands for the pseudo harmonic potential, for expressing the state of bounds data for chosen diatomic molecules (ScN, Cl_2, LiH, NO).The first notice isthe energy values increasing as the quantum numbers is raised. We also see that the energy of the molecule Cl_2 is the lowest, indicating its stability, and this agrees to the experimental data. When the energy is increased by supplementing the levels, the energy improves as the electrons migrate to a higher level, implying that the angular momentum increases as well. The results depending on quantum numbers n and l are reported. The boundary states indicated in this work with varying quantum quantities of n and l can be used to estimate the thermodynamic characteristics of the molecules with diatoms. The WKB approach has been used in this workto estimate the state of energy of quantum structures, and it is shown to have promise for other uses within the discipline of quantum physics.

Keywords: Schrodinger equation; bound states; WKB approximation; perturbed harmonic potential; energy spectrum.

EMPIRICAL MODELING OF TRANSITION METALNITRIDES (TMNs) PRECIPITATION IN ALLOYED STEELS

Abdelmalek ROULA

LIME-4; M. S. Benyahia Univ. Jijel; BP 98; Ouled Aissa; 18000, Algeria;
Corresponding Author: amkroula@univ-jijel.dz

Abstract

Enhancement of the superficial behavior of alloyed steel parts is the result of a change in their microstructural composition after carbides, nitrides, and/or carbonitrides precipitation. Transition metal nitrides (TMNs) are obtained after nitriding: a surface-hardening technique that triggers a local diffusion of nitrogen atoms into the material surface. Despite the presence of carbon (and/or sulfur) atoms, TMNs are the unique chemical combinations that appear at the end of such thermochemical treatment. In this study, an incisive combination of metallurgical processes theory fundamentals with rules of non-dimensional analysis allowed finding the Relative Nitriding Ability of any TM to form its nitride (denoted RNA^{M}_{Fe-C}) instead of any other chemicalcombination in alloyed steels. This empirical model is directly linked with the relative thermo- structural stability (RTSS) and the TMs electronegativity values that have been sorted to compute firstly, the nitriding Driving Force (DF) and secondly, the Total nitriding Retarding Force (TRF). The statistical analysis reveals a strong correlation of the RNA calculated values with the formation energy, the atomic number and the lattice parameter of its corresponding nitride. Manganese confirms to be the ablest element to form the most stable corresponding nitride (because of its high DF and Mn-N energy bonding values).

Keywords: Transition metals, nitrides, steels, statistical correlation.

STRUCTURAL PROPRIETIES, HIRSHFELD SURFACE ANALYSIS, RDG, HOMO-LUMO, MOLECULAR DOCKING OF 1-(4-FLUOROBENZYL)-5-BROMOLINDOLIN-2,3–DIONE

Sabrina SMATI*[1], Nouredine BOUKABCHA[1,2], Karima MENAD[1], Abdelkader CHOUAIH[1]

[1] Laboratory of Technology and Solid Properties (LTPS), University Abdelhamid Ibn BadisMostaganem, 27000, Mostaganem, Algeria,

[2]Chemistry Department, Faculty of Exact Sciences and Informatics, University Hassiba Benbouali, Chlef , 02000, Chlef, Algeria

Corresponding Author: sabrina.smati.etu@univ-mosta.dz

Abstract

Isatin and its derivatives find diverse applications in chemistry, medicine, and industry. In medicinal chemistry, they exhibit potential as drug intermediates with antimicrobial, antiviral, anticancer, and anti-inflammatory properties. Isatin derivatives are used in dye and pigment synthesis, forming metal complexes for catalysis, and as building blocks in synthetic chemistry. analytical chemistry, biological studies, and materials science. With their unique structure and reactivity, isatin derivatives remain valuable compounds for various research and practical applications

A combination of theoretical and experimental methodologies is used in this study to analyzeand understand the structural and vibrational properties of the title compound: FT-IR, UV-Vis, and 1 H and 13 C NMR chemical shifts utilizing the GIAO approach. The DFT approach was applied for all calculations, with the B3LYP functional and 6-311G(d,p) basis set. In the molecule, the HOMO-LUMO energy gap demonstrated a good charge transfer interaction. Hirshfeld surface analysis was used to examine the contribution of intermolecular interactions. The reduced density gradient (RDG) method was used to characterize and evaluate the nature of all possible interactions in our system, Then, molecular docking was used, which revealed good performance and binding affinity between the FBID molecule and the protein human serum albumin (HSA), which bears the code (2BXF).

Keywords: X-ray, Isatine, Docking, Hirshfeld, structure, RDG

ELUCIDATION DE STRUCTURE DE MOLECULE COMPLEXE « APPLICATION AUX ASPHALTENES »

CHERIFI Fatima Zahra

Department of Chemistry, Faculty of exact and applied science, Universityd'Oran1 AhmedBen Bella, B.P 1524 ,El M'Naouer -31000 Oran, Algeria
Corresponding Author: fatimazahracherifi@gmail.com

Abstract

molecular modelling now allows to give a good prediction and a good description of the properties of a given entity, these properties are related to the nature and shape of the molecule while experimental studies are not always easy to implement, it is therefore necessary to consider theoretical methods allowing to study more exhaustively and to confirm and complete the results of the experimental methods we proposed 18 structures of oil asphaltenes molecules of Hassi messaoud following work PhD students from the Laboratory of Macromolecular Physics (LCPM). A model structure was taken as a reference, and calculations were made on this structure using several methods of quantum-chemical calculations (semi-empirical, HF and DFT). Using the code Gaussian 09. The interpretation of the results allowed to see a clear increase of the energy with the increase of the length of the substituted aliphatic chain on the structure of the asphaltene, a more important increase is noticed also when an oxygen atom, nitrogen or sulphur is added; however substitution by the sulfur atom gives the highest energy compared to all substitutions this is due to the theoretical calculations of a structure are greatly related to the number of electrons of the whole molecule as well as the number of electrons of each atom. Based on our results we have concluded the DFT method using the correlation exchange function «B3LYP» with an average base of type 6- 31G it is the right choice.

Keywords: Molecular modelling ; asphaltene ; theoretical methods ; structures of oil asphaltenes quantum-chemical calculations .

SYNTHESE ET CARACTERISATION PHOTO PHYSIQUE ET ELECTROCHIMIQUE D'UN ENSEMBLE DE MOLECULES DE TYPE (PUSH-PULL) EN TANT QUE DOPANT POTENTIELPOUR UN SEMI-CONDUCTEUR A OXYDE MIXTE

Hanane BERDAA*[1,2], **M'hamed DJENNAD**[2,3]

[1] Faculty of Sciences and Technology, Tissemsilt University, Road of BOUGARA, Ben Hamouda, Tissemsilt 38004, Algeria
[2] Laboratory of SEAMM Faculty of Science and Technology, University of Mostaganem Abdelhamid Ibn Badis (UMAB), B.P. 188, Mostaganem 27000, Algeria
[3] Laboratory of Molecular and Thio-organic Chemistry (LCMT), CNRS UMR 6507, ENSICAEN, UNICaen & Univ. Normandy, 6 Bvd Maréchal June, 14050 Caen, France
Corresponding Author: anaberdaa2@gmail.com

Abstract

By varying the donor and acceptor groups, which are connected by a π spacer arm, we designed and synthesised a novel molecule with the donor spacer-acceptor compound 2f as a multifunctional component of fluorescence emitters in solution and 93% of yield. The proposed study aims to compare and quantify a set of push-pull type molecules of new linear conjugated systems with a variation of the acceptor force and a distance π between the donor and the acceptor for biological (biomedical) applications and materials in the field of semiconductors andphotocatalysis. The absorption spectrums of this molecule, as well as its fluorescence have been studied. Structure 2f was confirmed by means of single-crystal X-ray diffraction, 1HNMR, 13C- NMR, 19F-NMR, and mass spectroscopy. A series of new compounds, similar to a D-π-A, were also designed and synthesised, which show a high propensity for aggregation and crystallization (2e, 2g, and 2h) and increased the charge mobility in thin films. These push-pull organic molecules are formed from the electron-withdrawing functional groups (diester, diketone, bis- cyano, and hexafluoro-diketone), which are based on useful properties to improve the donor/acceptor interface, the optical absorption in the solution state, and the quantum yield. The photochemical properties of these compounds were studied using UV-Visible spectroscopy and fluorescence. The best dyes with having a yield of 26% (2g), 67% (2e), and 93% for (2f) showed NIR emission in solution state with an emission quantum yield of 14.5% at 627 nm, 1% at 570 nm, and 1% at 621 nm, respectively.

Keywords: Organic synthesis, donor-spacer-acceptor structure, electron transfer, supramolecular assemblies, Aggregation-induced emission (AIE)

ANALYSE COMPUTATIONNELLE DES CARACTERISTIQUES MOLECULAIRESD'UN NOUVEAU SEMI-CONDUCTEUR MOLECULAIRE THIAZOLIQUE

N. BELKAFOUF*[1], K. TOUBAL[2], A. CHOUAIH [1]

[1] Laboratoire de technologie et propriétés des solides (LTPS), Université de MostaganemAbdelhamid Ibn Badis, 27000 Mostaganem, Algérie
[2] Laboratoire de synthèse organique appliquée (LSOA), Département de chimie, Faculté dessciences, Université d'Oran 1 Ahmed Ben Bella, 31000, Oran, Algérie
Corresponding Author: nourelhouda.belkafouf@univ-mosta.dz

Abstract

Au cours de ces dernières années, L'analyse computationnelle des structures moléculaires organiques à base de groupement fonctionnel thiazolique ou ces dérivés est devenue un axe de recherche d'intérêt particulier dans le domaine optoélectronique et le domaine biologique. Cette analyse a été consacrée à déterminer plusieurs propriétés moléculaires serviront à caractériser et à fonctionnaliser les nouveaux matériaux organiques synthétisés. Dans ce contexte, nous nous intéressons à la détermination des propriétés physicochimiques d'un nouveau matériau thiazolique pour mettre en relation sa structure moléculaire à ses propriétés électroniques et optoélectroniques qui servent à fonctionnaliser ce matériau. Nous nous appuyons pour cela sur les résultats des analyses computationnelles des caractéristiques moléculaires déterminées sous le logiciel Gaussian 09, à l'aide de la théorie de la fonctionnelle de la densité (DFT), en utilisant la fonctionnelle hybride B3LYP et la base 6-311G (d, p).Le caractère semi-conducteur de la structure étudiée est confirmé par le calcul théorique à l'aide de la DFT de quelques grandeurs physiques comme l'énergie de réorganisation, les énergies des orbitales moléculaires frontières (HOMO et LUMO), la densité d'état électronique, le gap énergétique. Et le type de transfert de charge le plus dominant dans le matériau étudié est déterminé par l'énergie de réorganisation. D'autre grandeurs énergétiques sont calculées comme le potentiel d'extraction des électrons ou des trous, l'énergie de stabilisation des électrons ou des trous, l'électronégativité… Ces grandeurs sont utilisées généralement dans les tests des performances des dispositifs électroniques et optoélectroniques par la simulation numérique.

Keywords: Semi conducteur, thiazolique, Gaussian 09, DFT, gap.

ELECTRONIC AND SPECTROSCOPIC PROPERTIES OF TAUTOMERIC FORMS OF AN AZO DYE.

Mohammed Amin BENAOUDA & Mansour AZAYEZ

[1] *Department of chemistry Faculty of exact sciences and computing, University HBC, 02000,CHLEF, ALGERIA*
Corresponding Author: benaoudamine@yahoo.fr

Abstract

This work is dedicated to the study of electronic and spectroscopic properties of tautomeric forms of an azo dye, specifically the compound (E)-3-((2-nitrophenyl) diazenyl) pentane-2,4-dione. Geometry optimization calculations for the enol-azo and keto-hydrazone forms were carried out using Density Functional Theory (DFT). The TD-DFT method is employed to investigate the nature of electronic transitions by analyzing the absorption spectrum for each tautomeric form.

The overall picture of the obtained results reveals that the keto-hydrazone form is slightly less stable kinetically and more reactive, softer with a good electrophilic character in a more polar environment like DMSO, compared to the enol-azo form. The presence of the NO2 group in the ortho position of the benzene ring shifts the maximum wavelength towards higher values (bathochromic effect). This indicates that the choice of substituent can influence the absorption wavelength, thus achieving the desired color; this is the significance of substitution effects in dyes. In light of the results obtained in this study and considering the electrophilic nature of this dye, they could have industrial applications when involved in the formation of metal complexes.

Keywords: Azo dyes, optimization, Tautomeric forms, DFT (Density Functional Theory), NBO(Natural Bond Orbital), NLO (Nonlinear Optics).

EXPERIMENTAL AND THEORETICAL APPROACH OF ANORGANIC COMPOUND DETERMINATION AND GEOMETRY.

Nour Eddine BENHARKAT[*,1], Abdelkader CHOUAIH[2], Nourdine BOUKABCHA[1,2]

[1] Department of Chemistry, Faculty of Exact Sciences and Informatics, University of Hassiba Benbouali of Chlef, 02180, Ouled Fares, Algeria.

[2] Department of Chemistry, Faculty of Sciences and Technology, University of Abdelhamid Ibn Badis of Mostaganem, 27000, Mostaganem, Algeria.

Corresponding Author: n.benharkat@univ-chlef.dz

Abstract

An organic compound containing carbon, oxygen, nitrogen, and sulfur with the formula $C_9H_{13}N_3S_1$ has been further investigated using density functional theory (DFT) with the 6-31G(d, p) basis set to obtain optimized geometry. A good agreement is observed between the experimental XRD structure and the B3LYP optimized geometry. Structural investigation by single crystal X-ray diffraction analysis reveals that $C_9H_{13}N_3S_1$ crystallizes in a monoclinic system with space group $P2_1/c$, with an R-value of 7%. The unit cell parameters are a=9.4518(8) Å, b=8.3119(7) Å, c=13.4442(10) Å, α=90°, γ=90°, and β=97.559° (6). Furthermore, Frontier molecular orbitals (FMOs) analysis shows that the molecule contains acceptor and donor sites, and molecular electrostatic potential (MEP) analysis indicates that the title compound contains electrophilic and nucleophilic attack sites. These analyses have been performed at the B3LYP/6-31G (d, p) level to calculate the HOMO-LUMO gap. Finally, computational chemistry and experimental analysis show good agreement in various important data, indicating the potential for more productive future analyses and results in different fields.

Keywords: X-ray diffraction, DFT, Computational Chemistry, Theoretical Chemistry.

THEORETICAL INVESTIGATION OF HALOGEN'S EFFECT ON FERROELECTRICITY IN MULTI-LAYERED PHASES

Sarrah BENOMAR* & Hania DJANI

[1] *Faculté de chimie, Laboratoire de Chimie Théorique Computationnelle et Photonique, USTHB, B.P.32 El Alia, Bab Ezouar, Alger, Algérie*

Corresponding Author: benomar94sarah@gmail.com

Abstract

Using DFT calculations, we restrained the m=1 oxyfluoride Aurivillius Bi2TiO4F2 to adopt three ordered key configurations, such as tetragonal I4/mmm phases with fluorine anions distributed either at the octahedral apical sites or at the octahedral equatorial ones and orthorhombic Pma2 phase with fluorine anions distributed over both apical and equatorial sites. We explored the energetic of the metastable phases and their potential for ferroelectricity and found that the most favorable one is the mixture between apical and equatorial sites for fluorine. Phonon calculations performed via Abinit Package in the tetragonal I4/mmm with fluorine at the apical sites showed a strong c-axis polar instability Γ3-that co-exists with the ab-plane polar instability Γ5, commonly found in Aurivillius oxide phases. These two polar instabilities lead to Pc phase that displays in-plane and out-of-plane spontaneous polarizations as large as 44 µc/cm^2 and 35 µc/cm^2, respectively, which is unexpected in layered crystals. Opening new prospective design in thin films Aurivillius FeRam devices.

Keywords: Aurivillius, DFT, phonon, ferroelectric, polarization

CONTRIBUTION OF AN AMPEROMETRIC BASED BIOSENSOR FOR THEENZYMATIC DETECTION OF GLUCOSE

Bouhenna ABDESSLAM*[1], Oussama ZEGGAI[2,3], Mousaab BELARBI[4]

[1]Laboratory for Theoretical Physics and Material Physics, Department of Physics, Faculty of Exact Sciences and Informatics, Hassiba Benbouali University of Chlef, Chlef, Algeria
[2]Department of Common Core, Faculty of Exact Sciences and Informatics, Hassiba Ben BoualiUniversity, BP 151, Chlef 02000, Algeria
[3]Research Unit Materials and Renewable Energy (URMER), Abou Bekr Belkaïd University, BP119, Tlemcen, Algeria
[4]Laboratory of Micro and Nanophysics — LaMiN, Department of FPST - Ecole Nationale Polytechnique d'Oran-Maurice Audin, BP 1523, Oran 31000, Algeria
Corresponding Author: a.bouhenna@univ-chlef.dz

Abstract

Biosensors are a booming means of analysis. They are both rapid, selective and applicable to extremely varied fields (health, environment, agri-food, ... etc.). In this type of tool, a sensitive element of a biological nature (antibody, enzyme, microorganism, DNA, etc.) endowed with a power of recognition for an analyte or a group of analytes is associated with a transducer which may be of the thermal type, optical or electrochemical. New electrochemical sensors have been developed, given their high performance compared to other sensors. This work describes the characteristics of an electrochemical biosensor based on the amperometric technique to measure the glucose concentration in a sample using a ferri/ferrocyanide redox mediator in the presence ofthe enzyme glucose oxidase at the electrode level [1]. In this work describes the modeling of a blood glucose sensor using COMSOL Multiphysics, Chemical species interaction and diffusion of multiple bloode species produced a powerful working model used in developing and refining a range of blood glucose sensors for the commercial market.

Keywords: Biosensor; ferri/ferrocyanide; Glucose; COMSOL; electrodes.

EFFET DE REMPLACEMENT DU N2 PAR LE CO2 DANS L'AIR SUR LASTRUCTURE INTERNE ET LA FORMATION DES ESPECES POLLUANTES D’UNE FLAMME LAMINAIRE DE DIFFUSION

Mohamed Seghaier BRAKCHI*[,1], Saifeddine FAREH[1], Tarek BOUZZENADA[2]

[1]CMASMTF Laboratory, FSSA, Larbi Ben M’hidi University, Oum el Bouaghi, Algeria
[2]Environment Laboratory, Larbi Tbessi University - Tébessa 12000, Algeria
Corresponding Author: brakchimohamed1995@gmail.com

Abstract

La maîtrise de processus de combustion est essentielle, pour diminuer la consommation de combustible et les émissions polluantes. Pour l’atteindre, plusieurs études ont été lancées, parmi le préchauffage du comburant par le soutirage de la chaleur des produits de combustion qui sont une solution majeure à la diminution des dépenses d’énergie, et qui s’adapte bien à la combustion de gaz à faible pouvoir calorifique inférieur (PCI) ceci fait orienter les recherches vers de nouvelles technologies comme la combustion sans flamme. Le présent travail consiste à une analyse numérique de l’impact du remplacement d’une quantité d’azote de l’air par le dioxyde de carbone sur la structure interne et la production des espèces polluantes d’une flamme de diffusion laminaire à jet opposé d’un mélange biogaz/hydrogène-air dans un régime de combustion sans flammes avec un taux d’étirement constant $a=200s^{-1}$, la cinétique de combustion est décrite par le mécanisme GriMech2.1. La variation des paramètres influent directement sur la structure et la quantification des espèces polluantes, la réduction de l'oxygène a un effet très significatif sur la température et les émissions, un faible volume d'oxygène (4% - 8%) dans le flux d'oxydant chaud, caractérise la combustion sans flamme, l'augmentation de l’oxygène a un impact important sur la température et les émissions que la variation du mélange biogaz, l'augmentation de la dilution par CO2 dans le flux d'oxydant réduit la température et les émissions polluantes.

Mots clés : Biogaz hydrogéné, combustion sans flamme, taux de déformation, dilution par CO_2

CYCLO-OXYGENASE INHIBITOR DISCOVERY BASED ONCOMPUTATIONAL CHEMISTRY: MOLECULAR DOCKING, PHARMACOPHORE MAPPING, AND ADMET PREDICTIONS FROM PHYTOCHEMICALS

BOUKHATEM B.S. *, [1], BELHADJ A.E. [1], BOUKHATEM M.N. [2]

[1] *Laboratory of Biomaterials and Transport Phenomena, Faculty of Technology, University of Médéa, Algeria.*
[2] *Laboratory of Ethnobotany and Natural Products, ENS Kouba, Algiers.*
Corresponding Author: boukhatem.bouchra.sarah@gmail.com

Abstract

Cyclooxygenase (COX), the main protein receptor involved in prostaglandin production, is identified to take part in inflammatory reactions. COX inhibitors lack anti-thrombotic efficacy, which increases the risk of cardiovascular illnesses. This means that there is still a requirement for COX inhibitors with increased therapeutic effectiveness and tolerance. In recent years, the conventional medical system has paid a lot of interest to phytochemicals, secondarymetabolites and plant-derived essential oils (EO) from several aromatic herb species. In orderto minimize an overly inflammatory reaction, it is crucial to research how particular phytochemicals inhibit COX enzyme *in silico*. Therefore, the objective of the present research is to investigate the anti-inflammatory properties of plant-derived phytochemicals and to describe its mode of action using computational chemistry techniques. In this context, significant phytochemicals were subjected to molecular docking, pharmacophore modeling, and ADMET predictions in order to present scientific understanding into COX inhibition as well as to determine the most effectively powerful anti-inflammatory compounds. To investigate the binding affinity, hydrogen bond, and orientation of phytochemicals with COX protein, the molecular docking procedure was used. In order to evaluate the toxicity and drug-likeness ofthe test substances, ADMET profile (absorption, distribution, metabolism, excretion and toxicity) was predicted *in silico*. The oxygenated terpene pharmacophores and some reference anti-inflammatory drugs were presented using the ligand-based pharmacophore model. The outcomes of our computational work would set a standard for particular plant-based phytochemical produced from EO against COX inflammatory targets, thereby opening up new paths for the creation of inventive and more potent anti-inflammatory medications.

Keywords: *In silico* pharmacology, Computational chemistry, Computer-aided drug design, Molecular docking, Anti-inflammatory phytochemicals.

CRYSTAL STRUCTURE AND NONLINEAR OPTICAL PROPERTIES OF A NEWORGANIC COMPOUND

Samia DJABBOUR*[1,2]; Noureddine BOUKABCHA[2,3]; Souad BENNABI[2]; Khaled DRIM[1,2]; Noureddine BENHARKAT[1,2]; Abdelkader CHOUAIH[3]

[1] Laboratory Chemical Plant – Water – Energy, Hassiba Benbouali University, Algeria,
[2] Department of Chemistry, Faculty of Exact Sciences and Informatics, of Chlef, 02180, OuledFares, Algeria,
[3] Laboratory of Technology and Solid Properties (LTPS), Abdelhamid Ibn Badis University ofMostaganem, 27000 Mostaganem, Algeria.
Corresponding Author: s.djabbour@univ-chlef.dz

Abstract

A new organic compound 2-[(2, 4 Dimethoxy benzylidene)-hydrazono 1, 2-diphenyl-ethanone] (DBHDE) has been synthesized for the first time, and its structural characterization has been carried out using the X-ray diffraction method. The compound DBHDE crystallise in the P 2_1/c space group with Z=4 in the unit cell. It belongs to the monoclinic system with the following linear and angular dimensions: a=28.597(3) Å, b=8.2842(5) Å, c=17.8628(15) Å and β=107.925(6)°. To support the experimental results, density functional theory (DFT) calculations were performed using the B3LYP functional with a 6-311G (d, p) base set. All the theoretical results obtained are in perfect agreement with the experimental results. Furthermore, the non- linear optical (NLO) behaviour of DBHDE has been investigated by determining the electric dipole moment (μ_t), polarizability (α), first-order hyperpolarizability (β_t) and second-order hyperpolarizability (γ_t) using the same basis set. Finally, HOMO, LUMO, Gap, MEP and Mulliken charge investigations of the title molecule were performed.

Keywords: Crystal structure, DBHDE, XRD, DFT, NLO.

SYNTHESIS, DFT COMPUTATIONAL STUDIES ANDHOMO-LUMO OF NEW ORGANIC COMPOUND, SOLAR PHOTOVOLTAIC INVESTIGATION

Ahmed DJAFRI*,[1,2], Rachida RAHMANI[2,3], Abdelghani BOUCHAMA[1], Nadia TAIBI[1], Narimane NARIMANE[2], Soumia BELHACHEMI[2] and Abdelkader CHOUAIH[2]

[1] *Centre de Recherche Scientifique et Technique en Analyses Physico-chimiques (CRAPC), BP384-Bou-Ismail-RP 42004, Tipaza, Algérie*

[2] *Laboratory of Technology and Solid Properties (LTPS), Abdelhamid Ibn Badis University ofMostaganem, Mostaganem, Algeria*

[3] *Department of Process Engineering, Faculty of Sciences and Technology, Ahmed Zabana -University of Relizane, Relizane, Algeria*

Corresponding Author: djafahmed@yahoo.fr

Abstract

Faced with the scarcity of fossil fuels and global warming, it is becoming essential for humanity to find new sources of energy. The sun permanently provides the Earth with an inexhaustible source of energy, in quantity and almost everywhere on the surface of the globe.

A photovoltaic cell is an electronic component that, when exposed to light (photons), generates electricity. It is the photovoltaic effect that is at the origin of the phenomenon.

Our work objective is to synthesize a new low-gap heterocyclic organic compound based on thiazole and characterized by different spectroscopic methods (IR, NMR (^{1}H, ^{13}C)) and by X-ray diffraction on a single crystal. This last analysis allowed us to determine the three-dimensional structure of our product and to choose the most reliable theoretical calculation method. To determine the physicochemical properties of this organic compound, we used molecular modeling with the Gaussian program.

The theoretical calculation was carried out using the DFT method using the calculation base 6-31G (d,p). We also explored the charge distribution in the compound. The intramolecular charge transfer of this molecule mainly results from electronic transmission between the electron- donating and electron-accepting groups. The calculation carried out makes it possible to obtain the energy of the levels HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) and the energy of the Gap. The results obtained from the energy Gap show that our compound can be used in the production of photovoltaic cells.

Finally, this work can contribute to the development of the production of electricity from solar energy using organic molecules.

Keywords: Synthesis, thiazolidinone, DFT, HOMO- LUMO, photovoltaic cells

---

The First National Seminar on Chemistry (FNSC-1)

Sciences and Informatics Faculty, Hassiba Benbouali University of Chlef (Algeria), October 03-04, 2023

ELECTROSTATIC PROPERTIES DETERMINATION OF A NEW BENZIMIDAZOLE DERIVATIVE

Khaled DRIM*[1,2]; Youcef MEGROUSS[1,3]; M. DRISSI[3]; Abdelkader CHOUAIH[3]; Soumia DJABBOUR[1,2]; Noureddine BENHARKAT[1,2]

[1] Department of chemistry, Faculty of exact sciences and informatics, University Hassiba Benbouali University, Chlef, Postal code: 02180, City: Chlef, Country: Algeria
[2] Laboratory of Plant Chemistry - Water - Energy, Hassiba Benbouali University, Chlef [3] Laboratory of Technology and Solid Properties (LTPS), Faculty of Sciences and Technology, Abdelhamid Ibn Badis University of Mostaganem, Mostaganem 27000, Algeria
Corresponding Author: k.drim@univ-chlef.dz

Abstract

We present a comparative study based on the exploitation of high resolution X-ray diffraction experimental data on the one hand, and the oreticalab initio calculation son the other. We performed a detailed structural and the calculation of the electrostatic properties of the molecular system. The experimental determination of the crystal structure of the compound was carried out using high-resolution X-ray diffraction data. The general characteristic of the structure is the total planarity of the title molecule. In order to make a comparative study at the structural level, theoretical calculations using the density functional theory (DFT), implemented under the Gaussian 09 software, were carried out to model the molecular system composing our benzimidazole compound. Subsequently, physico-chemical analyzes by single crystal X-ray diffraction (DRX) and spectroscopic measurements (IR, NMR, UV-Visible) are carried out in order to identify the structure as well as the properties of our studied material. To obtain the electrostatic properties of the named compound: benzo[4,5]imidazo[1,2-c]thiazole-1(3H)-thione through theoretical calculations, we performed DFT calculations by using the (DFT/B3LYP) method with 6−311G(d, p) basis set.. The molecular dipole moment in the crystal was determined in order to understand the nature of inter and intramolecular charge transfer. In this context, the molecular electrostatic potential around the molecule and the HOMO-LUMO energy levels are also calculated, the orientation of the dipole moment has been determined in order to understand the nature of the inter- and intramolecular charge transfer. The comparison of the results shows a good agreement between the experimental values thus testifying to the goodquality of XRD data. The study revealed the nature of the intramolecular charge transfer existing within this molecule.

Keywords: Crystal structure, benzimidazole, DFT, X-ray diffraction, geometric parameters

IN SILICO ANALYSIS AND ADMET PREDICTION OFGINGEROL'S POTENTIAL AS A CYCLIN-DEPENDENT KINASE 2(CDK2) INHIBITOR IN CANCER

Mounir HAMMOUDI*,[1], Brahim FERAOUN[2], Khaled OTMANINE[3]

[1] *Laboratory of Biomaterials and Transport Phenomena (LBMPT), University of Medea,Algeria.*
[2] *Laboratoire Eau-Environnement (LEE), Faculty of Technology, Chlef, Algeria.*
[3] *Bio-Ressources Naturelles Locales (LBRN), Chlef University, Faculty of Technology,Department of Process Engineering, Chlef, Algeria.*
Corresponding Author: m.hammoudi@univ-dbkm.dz

Abstract

The Cyclin-Dependent Kinase 2 (CDK2) is an important cellular kinase involved in the regulation of the cell cycle and is frequently over expressed in various types of cancer. Inrecent years, natural compounds have garnered significant attention as potential anti-cancer agents. One such compound is gingerol, the primary pungent ingredient of ginger, which has been shown to possess diverse biological activities, including anti-inflammatory, antioxidant, and anti-tumor effects.

The present study aimed to investigate the potential of gingerol as a CDK2 inhibitor in cancer using in silico approaches. The compound was subjected to drug similarity prediction using DruLiTo and an ADMET prediction to assess absorption, distribution, metabolism, excretion, and toxicity using the online pkCSM tool.

The results of molecular docking simulations revealed that gingerol exhibits a higher binding affinity towards CDK2 compared to Roscovitine, with a binding energy of -5.3 kcal/mol and an inhibition constant (Ki) of 7714 nM. The study suggests that gingerol holds promise as a drug candidate due to its favorable pharmacokinetic properties and strong binding affinity to the target receptor CDK2. The molecular docking results imply that gingerol is the most potent inhibitor with a high affinity for the target receptor. Compliance with Lipinski and Veber rules also supports its potential as a drug candidate.

Keywords: CDK2, Gingerol, ADMET, Molecular Docking.

SPECTROSCOPIC CHARACTERIZATION, ELECTROSTATIC PROPERTIES STUDY AND HIRSHFELD SURFACE, OF COMPOUND ORGANIC USING DFT APPROACHES

Nawel KHELLOUL*[1,2], Rachida RAHMANI [2], Abdelkader CHOUAIH [2]

[1] Faculty of Science and Technology university of Mustapha Stambouli Mascara Algeria
[2] Laboratory of Technology and Solid Properties (LTPS), Abdelhamid Ibn Badis University ofMostaganem, Mostaganem , Algeria
Corresponding Author: nawelkhelloul@yahoo.fr

Abstract

We present the electron density analysis of organic compound (E)-3-(3,4-Dimethoxyphenyl)-1- (2-thienyl)prop-2-en-1-one with chemical formula C15H14O3S, it has two symmetry- independent molecules in the asymmetric unit with almost identical geometry.

Indeed, determining the electrostatic properties of nonlinear optical organic compounds. On the other hand, a structural analysis is performed. Two methods are used to obtain the structure, X- ray diffraction and theoretical calculation with density functional theory (DFT).

The Hirshfeld surface study is performed using the crystal program. The electrostatic potential and molecular dipole moment have been determined in order to understand the nature of inter- and intramolecular charge transfer. The study reveals the nature of intermolecular interactions including charge transfer and hydrogen bonds in the title compound. The molecule exhibits intermolecular hydrogen bond of type C–H…O. The HOMO and LUMO energy gap reveal that the energy gap reflects the chemical activity of the molecule from the results, the experimental value of the gap is in agreement with the theoretical value obtained by DFT/ B3LYP and which is 3 eV. These results show that the compound can possess photovoltaic properties. The dipole moment (μ), polarizability (α) and first hyperpolarizability (β) of the molecule have been reported. Finally, the cationic and anionic reactive sites of compound have been visualized on MEP surface.

Keywords: Hirshfeld Surface, electrostatic potential and hydrogen bond

THE NONLINEAR OPTICAL PROPERTIES OF PORPHYRINIC AND METALLOPORPHYRIN COMPOUNDS

Hicham MAHDJOUB-ARAIBI*,[1] & Mourad ZOUAOUI-RABAH[2]

[1] *Department of Chemistry, Faculty of Exact Sciences and Informatics Faculty, Universityof Hassiba BENBOUALI,02180, Chlef, ALGERIA.*

[2] *Department of Preparatory Education in Science and Technology, National PolytechnicSchool of Oran Maurice Audin.box B.P. 1523 Oran El M'Naouer, Oran, Algeria.*

Corresponding Author: hichammahdjoubaraib@gmail.com

Abstract

This work is focused on the quantum study of nonlinear optical properties (ONL) of some organic «Push Pull» molecules very elongated by the repetition of the same porphyrin unit. In addition, the improvement of ONL properties by the addition of a donor group that has a metallic character in order to have the ONL properties of the organometallic complex.

This study was carried out mainly by theoretical calculations using the DFT method by the functional CAM-B3LYP combined with the GENECP base.

The ONL results obtained by these calculations showed that the variation of the geometry by a position isomer has a significant effect on the ONL response and the prolongation of the chromophore chain per unit of (porphyrin) repeated gives very important improvements on the intramolecular charge transfer (ICT) evaluated by the power of attraction between the donor group and the acceptor.

The ONL results also showed an increase in the hyperpolarizability (β) of metalloporphyrins with a strongly conjugated structure.

Keywords: Nonlinear optic, DFT method, metalloporphyrins, hyperpolarizability.

ENHANCE LEAD BATTERY VOLTAGE VIA THE MULTI-ELECTROLYTES CONFIGURATION

Abdelmalek TAYEBI*, TELLI Laid, Larbi ZERROUALI

Laboratory inorganic materials, Department of chemistry, Faculty of science,University Mohammed Boudiaf M'sila, M'sila 28000, Algeria,

Corresponding Author: Abdelmalek.tayebi@univ-msila.dz

Abstract

The first rechargeable battery to be created was a lead-acid battery. It has undergone 164 years of evolution since French physicist Gaston Planté created it in 1859, for use as traction batteries, telecommunication batteries, backup power batteries, and starting batteries, among other things. Approximately 70% of the global secondary battery market's sales are of lead-acid batteries. They are seldom ever employed, nevertheless, in the portable field. The low energy density of cells is a product of both their capacitance and the applied voltage. A unique dual electrolyte structure was used to broaden the operating voltage range of these aqueous generators. An acid catholyte (pH≈0) and an alkaline anolyte (pH≈14) are created from a solid proton conducting material. During cell activity, the latter ensures electrical migration while preventing the two compartments of the cell from neutralizing the acid-base equilibrium. A novel rechargeable PbO_2-Pb battery system using Zn as negative and PbO_2 as positive electrodes in a KOH/H_2SO_4 dual-electrolyte is developed. Lead displays reversible electrochemical activity at the negative electrode in a strongly alkaline medium, simulating a rechargeable system. As a result, the electrode dropout recorded a voltage of -1.3 V/ESS. When employed in a multi-electrolyte cell with a PbO_2 electrode submerged in sulfuric acid, this electrode generates a 2.5 V electromotive force. As a result, the terminal voltage is 22% higher than it would be in a typical PbO_2/Pb cell. The theoretical capacity of the cell is increased by 18% with this battery chemistry.

Keywords: Lead-acid battery, energy density, dual electrolyte, electromotive force, theoretical capacity.

THEORETICAL STUDY OF BENZOHYDRAZIDE DERIVATIVES: DFTINVESTIGATION AND AIM ANALYSIS

Fatima YAHIA CHERIF* & Nadia BENHALIMA

Department of Chemistry Faculty of Sciences University of Saida – Dr Moulay Tahar, 20000, Saida, Algeria,
Corresponding Author: yc_fatima@yahoo.fr / fatima.yahiacherif@univ-saida.dz

Abstract

The hydrazide and benzohydrazide derivatives are very interesting compounds because they exhibit good biological activities. They are known by their various activities such as antituberculous, antimicrobial, anticonvulsant, anti–inflammatory, antidepressant, analgesic, antiplatelet, anti–HIV and even anti–tumor activities. The benzohydrazide derivatives with both electron donor–acceptor groups connected through a π–conjugation bridge provide a pathway for the redistribution of the electron density under the influence of an external field. These compounds are of great importance in material chemistry owing to their strong chemical stability, and they are considered attractive candidates for optoelectronic technologies. No X–ray studies ofthe above compounds under study have been reported until now. The aim of the present work is to carry out a theoretical study of the structures of benzohydrazide derivatives using density function theory (DFT) methods. The HOMO–LUMO energy gaps and the global chemical reactivity descriptors were computed by B3LYP and CAMB3LYP using 6–31G (d,p). Besides, the stability and charge delocalization were studied by natural bond orbital analysis. Topological analyzes such as atom in molecule (AIM), natural bonding orbital (NBO) and molecular electrostatic potential (MEP) have used to compute intermolecular interactions and in particular hydrogen bonds. Our results revealed that the most important charge transfer interaction energies were mainly attributed to the orbital overlap between $n3$ (O11) and π^* (N9–O10) with stability energy of 228.59 *kJ/mol*. The HOMO energy level of all compounds was found within the range extending from –6.15 to –6.47 (*eV*), whereas the LUMO was in the range of –2.55 to –2.70 (eV). These data suggest that the molecule requires only a small energy to change state from HOMO to LUMO. The energy gap ΔE in the range from 3.63 to 3.92 (eV) indicates that our compounds possess good chemical stability and reactivity.

Keywords: Benzohydrazide, Analyse AIM, Analyse NBO, Analyse MEP

CHARACTERIZING THE ELECTRONIC AND OPTICAL PROPERTIES OF SMALL MOLECULAR SEMICONDUCTORS FOR APPLICATION IN THIN-FILM ORGANIC TRANSISTORS USEDIN PHOTOVOLTAIC SOLAR CELLS.

Roquiya Nour El Houda ZORGANI*, Fouad LEBSIR, Farouk Hamza REGUIG Mohammed Aymen ZORGANI

Laboratoire de Chimie Physique Macromoléculaire, Université d'Oran 1 Ahmed Ben Bella, Es-Sénia, Oran, ALGERIE

Corresponding Author: zornour@outlook.fr

Abstract

Organic Thin Film Transistors (OTFTs) represent a fascinating class of electronic devices that have gained significant attention due to their potential applications in flexible and wearable electronics, displays, sensors, and more. Unlike traditional silicon-based transistors, OTFTs utilize organic materials as the active semiconducting layer, offering unique advantages such as mechanical flexibility, low-cost manufacturing processes, and the ability to create large-area devices on various substrates.

To study the properties of these organic molecules, calculations were performed using Gaussian, a software for molecular modeling and computational chemistry studies. Density Functional Theory (DFT) employing the B3LYP hybrid functional was utilized to determine electronic properties, including the energies of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), the band gap width, chemical potential, and electronegativity, among others. Time-Dependent Density Functional Theory (TD-DFT) was employed to ascertain optical properties such as excitation energy and absorption wavelength.

In summary, these studies and calculations provide valuable insights into the electronic and optical characteristics of small organic molecules. This knowledge contributes to the design and advancement of efficient photovoltaic materials for applications in the field of renewable energies.

Keywords: Thin film transistors , DFT,TD-DFT, photovoltaic.

THE INVESTIGATION OF THE CONFORMATION AND REACTIVITY OF ALGINATES USING DFT CALCULATIONS

Rabah Mourad ZOUAOUI*[1, 3]; Hicham MAHDJOUB-ARAIBI[2, 3]

[1] Department of Preparatory Education in Science and Technology, National Polytechnic School of Oran Maurice Audin.box B.P. 1523 Oran El M'Naouer, Oran, Algeria.
[2]Departement of Chemistry, Faculty of exact Sciences and informatics, Hassiba Benbouali University, Chlef, P.O. Box 78C, Ouled Fares Chlef 02180, Algeria.
[3]Laboratory of Materials chemistry catalysis and reactivity, department of Chemistry, Faculty of exact Sciences and informatics, Hassiba Benbouali University, Chlef, P.O. Box 78C, Ouled Fares Chlef 02180, Algeria.
Corresponding Author: crmamourad@yahoo.fr / rabah-mourad.zouoaui@enp-oran.dz

Abstract

The lower energy conformers of four disaccharides found in alginic acids, namely MM, GG, MG, and GM, based on β-D-mannuronic (M) and α-L-guluronic acid (G), were determined using isoenergetic maps generated through the density functional theory (DFT) method with the B3LYP/6-31G(d,p) level of theory. These preferred structures were then combined with monovalent cations (Li+, Na+, and K+) and fully optimized. Additionally, an isoenergetic map was created for the complex (MG^{2-},$2Na^{+}$). The reactivity of MG complexes with mono- and bivalent cations was investigated using the global nucleophilic index, and the position selectivity was predicted using the local nucleophilic indices. The empirical indices of reactivity successfully predicted the experimental trends of relative reactivity and regioselectivity of the complexes. The regioselectivity study showed that the nucleophilic attacks occur on the carboxylic groups or on cations. Finally, the HOMO/LUMO and MESP analyses confirmed these deductions and were in agreement with reactivity studies.

Keywords: DFT method, $\Delta_{H\text{-}L}$, Alginic acids, Monovalent and Divalent cations, conformers.

X-RAY CRYSTAL STRUCTURES AND DFT CALCULATIONS OF A BENZOTHIAZOLYL-COUMARIN HYBRID COMPOUND

Sid Ahmed KAAS*,[1] & Youcef MEGROUSS[2]

[1] Department of Material Science, Faculty of Science and Technology, Tissemsilt University,3800, Tissemsilt, Algeria,
[2] Department of Chemistry, Faculty of Exact Sciences and Informatics, Hassiba BenboualiUniversity, Chlef, 02000 Algeria
Corresponding Author: kaas.sid.ahmed@univ-tissemsilt.dz

Abstract

Benzothiazole and its derivatives are significant heterocyclicaromatic compounds. The benzothiazole moiety is giving rise to a category of compounds with several applications in medication and in nonlinear optics. Heterocyclic molecule based benzothiazole derivatives exhibit strong fluorescence and luminescence in the solid state and in solutions. Coumarins have been well studied as a distinct construct for mapping novel agents that have great attractiveness and specificity for diverse molecular targets of antiviral agents. The present study explained the structure and the geometry of benzothiazolyl-coumarin derivatives (N-[3-(benzo[d]thiazol-2-yl)- 6-bromo-2H-chromen-2-ylidene]-4-methylbenzenamine) using X-ray results and DFT calculations. The $C_{chromene}$ N—C angle is wide [125.28°]. The benzothiazole and chromene ring systems are almost coplanar. the toluene ring system is rotated by ca 40° out of the chromene plane. the B3LYP/6-311G(d,p) theoretical level of theory was used to optimize the quantum mechanical calculations of the geometrical characteristics and energy of The compound, $C_{23}H_{15}BrN_2OS$under study. Also, the distribution of electron density, followed by an analysis of the electrostatic potential of the molecule was studied.

Keywords: Benzothiazolyl-coumarin derivatives, DFT, distribution of electron density, MEP.

FIRST PRINCIPLES CALCULATIONS OF STRUCTURAL, ELASTIC ANDELECTRONICPROPERTIES OF HALF-HEUSLER CoYSn COMPOUND

Y. SEFIR*[,1], S. TERKHI[1], N. MEHTOUGUI[2], A. ZITOUNI[1], B. BOUADJEMI[1]

[1]*Laboratory of Technology and of Solids Properties, Faculty of Sciences and Technology,BP227 Abdelhamid Ibn Badis University, Mostaganem 27000, Algeria*
[2]*Laboratory of Elaboration and Characterization Physical Mechanics and Metallurgical of Material ECP3M, Faculty of Sciences and Technology, BP227*
Abdelhamid Ibn Badis University, Mostaganem 27000, Algeria
Corresponding Author: sefiryamina@hotmail.fr / yamina.sefir@univ-mosta.dz

---

Abstract

First-principles calculations are performed to investigate the structural, elastic and electronic properties of the half-Hesuler alloy CoYSn in three phases (*I*, *II* and *III* phases) by using the full-potential linearized augmented plane wave (FP-LAPW) [1] as implemented in the WIEN2k [2] code based on the density functional theory (DFT), within the (GGA). From the structural properties, we have calculated the equilibrium lattice constants, the bulk modulus andthe pressure derivative of the bulk modulus and the total energy as functions of the volume for the three phases (*I*, *II* and *III*). We have found that the compound is most stable in the phase *II*, and have a ferromagnetic state at optimized lattice constants. Also, we have calculated the electronic properties of the half-Heusler alloy and shown that the compound have metallic characters. The elastic constants, such as the shear modulus, Young's modulus, anisotropy factor and Poisson's ratio, have been obtained and demonstrate that the compound is ductile, anisotropic and stiff.

Keywords: Cubic ferromagnetic half-Hesuler, FP-LAPW method, electronic structure, elastic properties.

STRUCTURAL RELATIONSHIP WITH NONLINEAROPTICAL PROPERTIES OF AN ISATIN DERIVATIVE.

Mohammed HADJ MORTADA BELHACHEMI*[,1], Nourdine BOUKABCHA[1,2], Abdelkader CHOUAIH[1]

[1] *Department of Process Engineering, Faculty of Science and Technology, University of Abdelhamid Ibn Badis, 27000, Mostaganem, Algeria,*

[2]*Department of Chemistry, Faculty of Exact Science and Informatics, University of Hassiba BenBouali, 02000, Chlef, Algeria,*

Corresponding Author: belhachemi.mortada@yahoo.com

Abstract

Non-linear optics has become a promising area of research for scientists and researchers due to the possibility of manipulating light waves and generating new wavelengths. Organic compounds such as isatin and its derivatives are good candidates with remarkable optoelectronic and NLO properties. The importance of the ONL properties of molecules depends on their hyperpolarizability. The aim of the present study is to investigate the relationship between polysubstituted molecule structure and their ONL activity. The molecule studied here is 1-(4-fluorobenzyl)-5-bromolindolin-2,3-dione (FBID). In this work, we assessed the effects of substituting fluorine, chlorine and bromine atoms in the para, meta and ortho positions of this molecule on its ONL properties. these properties of these molecules are investigated using quantum chemical calculations with GAUSSIAN software, enabling us to calculate dipole moment, polarizability and first-order hyperpolarizability employing the density functional theory (DFT) method, the B3LYP functional and 6-311G(d,p) basis set. Based on the results, in comparison with the other nine structures, the ortho-Br position displays the highest value of dipole moment. As far as first-order hyperpolarizability is concerned, the molecule substituted by the bromine atom in the para position reveals maximum value. In conclusion, all the nine structures possess nonlinear optical properties, in particular the molecule substituted by the Bromine atom in the para position.

Keywords: Halogens, Substitution, NLO, Dipole moment, Hyperpolarizability.

THERETICAL STADY OF STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF CHALCOGENIDE COMPOUND MN_2SIS_4

H. BOUHANI BENZIANE*[,1,2] & M. SAHNOUN[2]

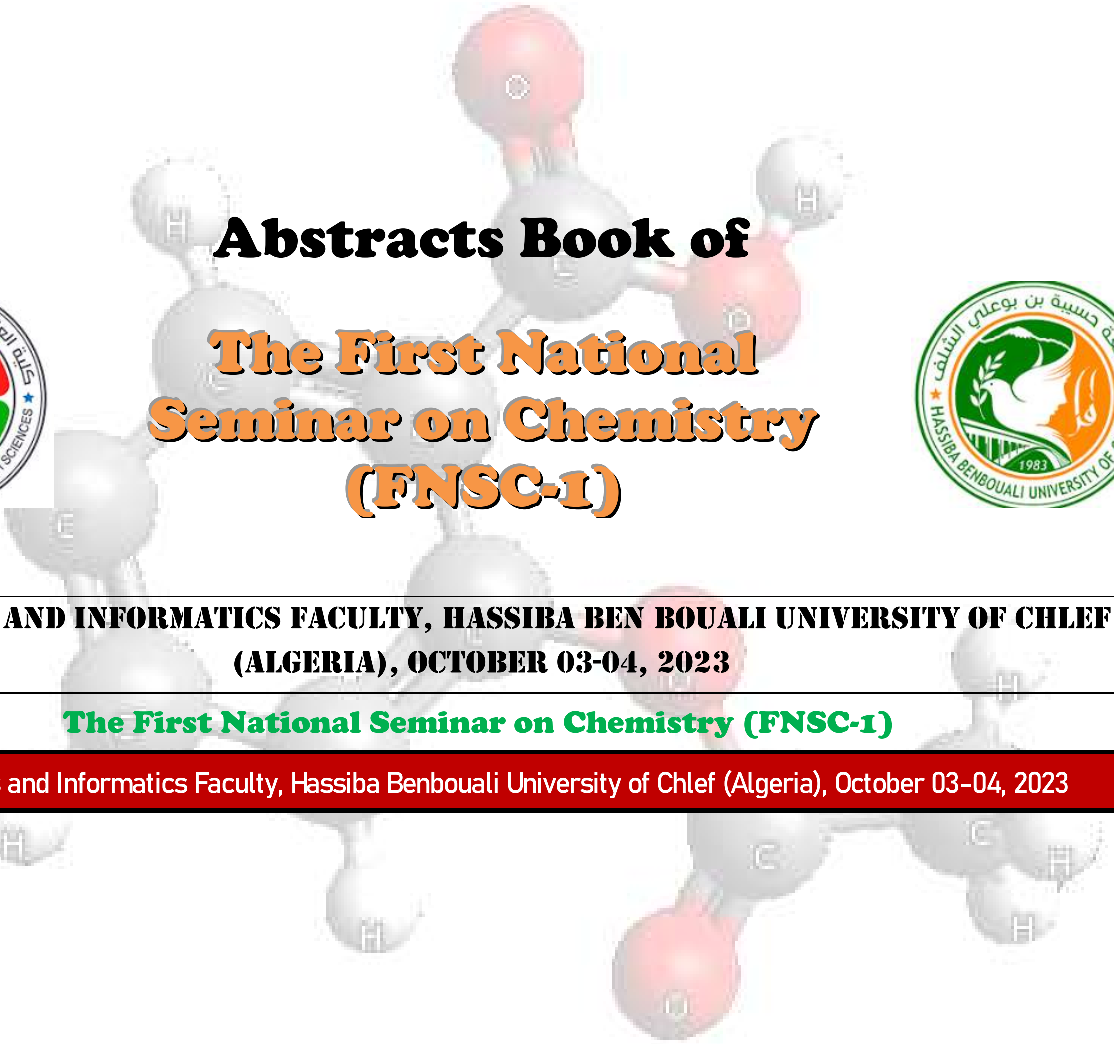
[1] Exact Sciences Faculty, Hassiba Benbouali University of Chlef , Chlef, Algeria.
[2] Laboratoire de Physique Quantique de la Matière et Modélisation Mathématique (LPQ3M),University Mustapha Stambouli of Mascara, Algérie
Corresponding Author: h.bouhanibenziane@univ-chlef.dz

Abstract

Mn_2SiS_4 belongs to the adamantine family of quaternary chalcogenides crystallizing in the olivine type structure, which can be described from a hexagonal close-packing of sulfur anions with the octahedral and tetrahedral sites occupied by the Manganese and Silicon cations, respectively. In this work , structural, electrical and magnetic properties of Mn_2SiS_4 were studied by using Full Potential Linear Augmented Plane Wave (FP-LAPW) based on density functional theory. Perdew Becke Ernzerhof (GGA-PBE) and modified Becke-Johnson exchange potential (MBJ) were used for the exchange correlation potential. The results on the basic physical parameters, such as the lattice constant, bulk modulus, pressure derivative of bulk modulus, were presented. Band structures and density of states were calculated and it was found that the crystal is a semiconductor with a direct energy band gap of about 1.34 eV for Mn_2SiS_4.

Keywords: Electronic structure, magnetic properties, ab-initio calculation, spintronics, olivine

Revue Nature et Technologie
Academic Journal Edited By Hassiba BENBOUALI University
of Chlef (Algeria) under ISSN : 1112-9778
https://journals.univ-chlef.dz/index.php/natec/



Abstracts Book of

The First National Seminar on Chemistry (FNSC-1)

SCIENCES AND INFORMATICS FACULTY, HASSIBA BEN BOUALI UNIVERSITY OF CHLEF (ALGERIA), OCTOBER 03-04, 2023

The First National Seminar on Chemistry (FNSC-1)

Sciences and Informatics Faculty, Hassiba Benbouali University of Chlef (Algeria), October 03-04, 2023