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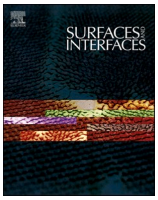

Synthesis and theoretical studies of novel conjugated polyazomethines and their application as efficient inhibitors for C1018 steel pickling corrosion behavior

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ABSTRACT

The idea of the existing work is to progress the preparation of four conjugated polyazomethines contained thiazole through the backbone of the polymer. The synthesized conjugated polyazomethines were categorized and assessed as novel inhibitors for the C1018 steel pickling corrosion behavior at 298–328 K using surface morphology of C1018 steel electrode, potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS). The assessed polymers performed as effective inhibitors for C1018 steel corrosion in pickling solution. The protection capacity of the polyazomethines augmented with a rise in concentration to attain 98.2% efficacy with 150 mg L^{-1} at 298 K. PDP plots designated that the conjugated polyazomethines performs as mixed-type inhibitors and adsorbed on the C1018 steel interface via chemisorption. Isotherm model of Langmuir was found the preeminent mode for the adsorption of polymers. The surface morphology examinations established the development of a protective layer getting a thick coverage at the optimal dose. Moreover, theoretical study of Monte Carlo (MC) simulations and density functional theory (DFT) were used to govern the association among protection capacity and molecular structure. This study could be provided novel polyazomethines inhibitors for C1018-steel corrosion protection in different industrial environments, especially in the pickling solution.

1. Introduction

C-steel (carbon steel) has been chosen as unique of the greatest significance and extensively utilized structural accessories in numerous industries, including automotive, chemical processing water, petroleum, and power generation, and a diversity of other applications [1,2]. The wide and important use of C- steel is related to its outstanding mechanical features and low-cost [2,4]. Nevertheless, C-steel is inclined to corrosion in refinery categorized mineral acids such as H_2SO_4 (sulfuric acid), HCl (hydrochloric acid), H_2SO_3 (sulfurous acid), and thiosulfurous [5]. Among the previous corrosion mediums, hydrochloric acid is generally used in various industrial implementations like acid pickling, industrial cleaning, scale and rust elimination, acidification of oil wells in petrochemical procedures, and oil retrieval at temperatures up to 333 K [6].

With the aim of treat the aggressive attack of these acids, inhibitors are introduced to the corrosive medium, which diminishes the aggressiveness of acids to the C-steel surface. The chemical materials with both inorganic and organic sources have been applied as inhibitors to preserve minerals from harsh solutions [7]. Organic molecules containing hetero-atoms like nitrogen, oxygen and sulfur, and aromatic rings π-electrons are originated to be actually effective in quashing the corrosion of the metal in various mediums [8,9]. Among the carbon-based materials, polymeric corrosion inhibitors are a very wide choice owing to their huge efficient groups and their capability to complex with metal ions at interfaces [10,11]. By covering great surface extents of alloys and metals in the corrosive solutions, these formed pincers effectively "complete" the surface from aggressive ions and molecules attack thus contributing the required inhibition [12]. Additionally, small inhibitor molecules incline to destroy at higher

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Research Article

Synthesis of an optimized ZnS/Au/ZnS multilayer films for solar cell electrode applications

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ABSTRACT

In this study, different film constructions (ZnS, ZnS/Au, and ZnS/Au/ZnS) were evaporated by thermal-evaporation. The study was conducted in order to identify the best film for solar cell applications. The study identifies ZnS (399.6 nm)/Au (18 nm) as the most appropriate film for further investigation because it shows a maximum optical band gap ≈ 3.43 eV and the minimum resistivity (0.46 × 10^{-3} Ω cm). It is noticed that the interference fringes disappeared due to the addition of the Au layer. The absorption edge was shifted towards a lower energy as the Au increased. The band gap E_g and resistivity ρ_{Rt} were 3.49 eV and 0.12 × 10^{-3} Ωcm respectively. The refractive index increased up to the maximum value 6.2. The ZnS (399.6 nm)/Au (6 nm)/ZnS (399.6 nm) films exhibited amorphous structure, and with the increase of the Au thickness layer, the diffraction peaks related to FCC phase of the Au appeared. The film ZnS (399.6)/Au 18/ZnS (399.6) shows very promising parameters. The bandgap Eg is 3.38 eV, the sheet resistance is 1.53 × 10^{-3} Ω, the figure of merit equals 3.7 × 10^{-3} Ω^{-1} and the refractive index is 6.20. The results prove that the film ZnS (399.6)/Au 18/ZnS (399) is suitable for conductive electrodes in solar cells.

1. 1- Introduction

Transparent conduction oxides (TCO's) have been used for the optoelectronic systems applications such as; photovoltaic solar cell, electro-chromic equipment and transistors [1–6]. A synthesis of indium tin oxide, by sputtering, is not easy because of the behavior of indium ions during the diffusion process; high electrical resistivity; scarcity and the high cost of indium resources in nature [7–9]. It is urgently needed to find low cost TCO's for commercial applications [10]. Placing metal between two dielectric layers (dielectric/metal/dielectric (D/M/D)) enhances the reflection of metal in the visible region. This arrangement causes more perfect electrical and optical characteristics than a single layer TCO's [4,11–16]. Extensive attempts have been done mainly on the multi-layers structure, (AZO/Au/AZO [17,18], ITO/Au/ITO [19,20], ZnS/Ag/ZnS [15,16], ZnO/Au/ZnO [21], SnO_2/Ag/SnO_2 [22], ZnO/Cu/ZnO [23] and ZnS/Au/ZnS [24]).

AZO/Au/AZO multi-layers were deposited, by magnetron sputtering, on glass substrate at various Au thicknesses 5–20 nm. Chien Hsun ehu reported that the best values of the mobility and the free carrier concentration were 1.01 × 10^{-5} Ω cm, 2.7665 $cm^2v^{-1}s^{-1}$, and 4.563 × 10^{22} cm^{-3} respectively. The transmittance was 86.18% at 650 nm wavelengths at a thickness of 8 nm [17]. Seung jun Lee et al. prepared the AZO/Au (0–12 nm)/AZO multi-layers by atomic layer deposition (ALD) and electron beam evaporation technologies. As the thickness of the Au increases, the free carrier concentration increases to 4.2 × 10^{21} cm^{-1}. The resistivity decreased from 2.6 × 10^{-3} to 1.2 × 10^{-4} Ω cm and the transmittance decreased from 80% to 48% [18]. The ITO/Au (10 nm)/ITO multi-layers thin films were deposited on poly-carbonate substrate [19]. For single layer ITO, the free carrier concentration was 7.12 × 10^{22} and increased to 3.26 × 10^{22} cm^{-3} for ITO/Au/ITO [20]. Xuanjie Liu et al. (2001) prepared ZnS/Ag/ZnS nano-multilayers by a thermal evaporation technique. The sheet resistance of ZnS/Ag/ZnS was 3 Ω/cm^2 and the figure of merit F_{TC} was 7.3 × 10^{-2} Ω^{-1} [25]. The physical properties of the ZnO/Au (3 nm)/ZnO have been studied by H. M. Lee. The transmittance of the thin films decreased because of the addition of Au layer [21]. Caifeng Wang and Bo Hu synthesized ZnS/Au/ZnS multi-layer on quartz glass substrates. They reported that the maximum optical transmittance increases to 86.2% at 200 °C [24].

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Synthesis of highly crystalline $LaFeO_3$ nanospheres for phenoxazinone synthase mimicking activity†

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$LaFeO_3$ nanospheres with an orthorhombic perovskite structure were synthesized by a sol–gel autocombustion method in the presence of different citric acid ratios ($x = 2$, 4, 8, and 16) and utilized for the photocatalytic conversion of *o*-aminophenol (OAP) to 2-aminophenoxazine-3-one (APX) for the first time. OAP is one of the most toxic phenolic derivatives used as a starting material in many industries; however, the dimerization product APX has diverse therapeutic properties. Photocatalytic conversion was carried out in ethanol/water and acetonitrile/water mixtures in the absence and presence of molecular oxygen at ambient temperature *via* the oxidative coupling reaction that mimics phenoxazinone synthase-like activity. The $LaFeO_3$ samples showed a superior photocatalytic activity of OAP to APX with rate constants of 0.43 and 0.92 min^{-1} in the absence and presence of molecular oxygen, respectively. Thus, the $LaFeO_3$ nanozymes could be used as promising candidates in industrial water treatment and phenoxazinone synthase-like activity.

1. Introduction

Millions of tons of organics are intensively consumed in food additives, pharmaceuticals, pesticides, painting, dying, textile industries, and agricultural activities every year. Most of these undesired reagents or starting materials, particularly those called persistent contaminants, are subsequently discharge in the environment and cause serious health risks.[1] Considering the environmental safety issues and energy-effective cost, many restrictions are assessed recently on chemical industries to switch and utilize alternative or greener manufacturing routes. However, large amounts of persistent organic contaminants are still discharged. Biological, thermal, physical, and chemical treatment technologies have been adopted for the mitigation of organics in the last decades.[2–4] Several microorganisms are being utilized to degrade biodegradable organics but the process usually takes a long retention time. Thermal treatment also consumes a large quantity of energy. Membrane separations and adsorption are widely used for removing organic contaminants.[5,6] Functional materials with large surface areas should be engineered and developed. However, a long separation time and surface regeneration with stable functionality are still major obstacles. Among the aforementioned technologies, chemical oxidation is a promising process for large-scale wastewater treatment under mild conditions. It is usually carried out using chemical reagents, which might be homogenous or heterogeneous processes. Thus, many research works have been devoted to develop both homogenous and heterogeneous catalysts for efficient wastewater treatment.[7,8]

The photocatalytic oxidation process is an efficient and eco-friendly methodology that utilizes light energy to drive the oxidation reaction, leading to the degradation of organic contaminants to low molecular oxygenated chemical species or the synthesis of new compounds.[9,10] Irradiation of a semiconductor with a light stimulates the transfer of electrons in the valence band (VB) to the conduction band, leaving behind a positive charge carrier known as a hole.[11] These photo-generated charge carriers (e^-/h^+) might be recombined again in the bulk catalyst nanoparticles, producing thermal energy or migrating to the catalyst surface. The surface charge carriers can further participate in the catalytic reaction through their redox potentials. The photo-generated hole acts as an electron acceptor in the oxidation processes. Alternatively, the surface adsorbed species such as H_2O molecules and OH^- group may trap the photo-generated holes, producing hydroxyl radicals ($^{\bullet}OH$), which is a non-selective strong oxidizing species with a redox potential of 2.80 V (*vs.* NHE). On the other hand, the electrons in the conduction band might reduce the adsorbed O_2 molecules and form superoxide $O_2^{\bullet-}$ radicals. Metal oxides such as TiO_2 and ZnO have been commonly used as heterogeneous photocatalysts.[12] However, their wide energy band gap requires a high photo-energy for excitation. Regrettably, UV irradiation represents only less than 5% of solar energy, which limits these metal oxides' applicability. Accordingly, various attempts have been undertaken to make the photocatalysis process more efficient and economical by utilizing a wide range of visible-light energy.

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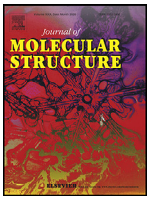

Synthesis, characterization, molecular modeling and preliminary biochemical evaluation of new copper (II) mixed-ligand complexes

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ABSTRACT

Three new Cu(II) mixed-ligand complexes of the type [Cu(primary ligand)(secondary co-ligand)], were synthesized, characterized and preliminary tested for their biochemical activities. The primary ligand (HL) was derived from condensation of p-toluidine with 2-hydroxy-naphthalhyde. Three different N-heterocyclic compounds, 8-hydroxy-quinoline (HQ), 2-(1H-benzimidazol-2-yl)phenol (HB), and 2-(4,5-diphenyl-1H-imidazol-2-yl)phenol (HI), were used as secondary co-ligands. Inhibitory capacity of the synthesized compounds were screened against the growth of pathogenic bacteria [*E. coli* (G^-) and *B. cereus* (G^+)] and fungi (*A. fumigatus*), in terms of inhibition zone (IZ, mm), and minimum inhibitory concentration (MIC, μg/mL) using the disc diffusion method. Furthermore, the complexes were tested for their phenoxazinone synthase-like activity in terms of K_{cat}. Density functional theory (DFT) calculations based on B3LYP with LanL2DZ level of theory were performed to prove the proposed geometry of the complexes as well as evaluate the electronic parameters responsible for their reactivity. Structure activity relationship formula was derived by correlating the experimental data (MIC or K_{cat}) with the calculated electronic parameters.

1. Introduction

Copper plays a considerable biochemical role either as an essential trace metal or as a constituent of various external administered compounds in humans. In the former role, it is bound to albumin, and other proteins, while in the latter, it is bound to many ligands forming complexes that interact with biomolecules, mainly proteins and nucleic acids [1]. Current interest in Cu complexes is due to their diverse biological significance as antimicrobial, antiviral, anti-inflammatory, antitumor agents, and enzyme inhibitors [2,3].

The copper-containing metalloenzymes play an important catalytic role in living systems as dioxygen and substrate activators toward different bio-functions, e.g. Phenoxazinone synthase activity [4,5]. Phenoxazinone synthase, is a multicopper oxidase enzyme, found naturally in the bacterium, Streptomyces antibiotics, which catalyzes the oxidative coupling of o-aminophenol (OAP) derivatives into phenoxazinone chromophore (Phz). The latter is used clinically for the treatment of Wilm's tumor, gestational choriocarcinoma, and other tumors in which phenoxazinone chromophore is recognized to inhibit DNA-dependent RNA synthesis by intercalation to DNA [6].

There has been enhanced interest in developing new Cu(II) complexes for their biochemical significance. Thus, in the present framework, three Cu(II) mixed-ligand complexes involving a Schiff base as the primary ligand, and N-heterocyclic co-ligand as the secondary one, had been prepared and characterized. Additionally, a preliminary investigation of their *in-vitro* antimicrobial and phenoxazinone synthase-mimicking activity was evaluated. A preliminary screening was undertaken to test their activity efficacies against economically important fungi and bacteria. Firstly, the bare ligands, and their complexes have been evaluated against pathogenic bacteria and fungi that are common contaminants of the environment, and some of which are involved in human and animal diseases, e.g. *Aspergillus fumigatus*, or frequently reported from contaminated soil, water and food substances, e.g. *Escherichia coli* (G^-) and *Bacillus cereus* (G^+). Also, their catalytic activity towards the oxidative coupling of OAP had been investigated.

2. Experimental

2.1. Synthesis

All Chemicals used in synthesis of the investigated compounds were of analytical grade and used as received without further purification.

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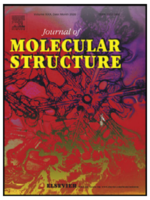

Synthesis, crystal structural determination and *in silco* biological studies of 3,3′-ethane-1,2-diylbis(2-benzylidene-1,3-thiazolidin-4-one

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ABSTRACT

A new thiazolidine derivative, 3,3′-ethane-1,2-diylbis(2-benzylidene-1,3-thiazolidin-4-one (**4**) was synthesized and the product obtained was characterized by NMR, IR and mass spectral studies, and the structure was confirmed by single crystal X-ray diffraction studies. The title compound crystallizes in the monoclinic space group $P2_1/n$, the unit cell parameters are $a = 15.9505(8)$ Å, $b = 6.6818(3)$ Å, $c = 18.1799(9)$ Å, $\beta = 94.249(2)°$ and Z = 4 at 150 K. In the title molecule, $C_{20}H_{18}N_4O_2S_2$, the thiazolidine rings adopt a "pincer" conformation with the phenylimino substituents extending outwards on both sides. A layer structure is formed in the crystal by C—H···N and C—H···O hydrogen bonds. A Hirshfeld surface analysis was used to explore the nature of the intermolecular interactions in the crystal structure employing molecular surface contours and 2D fingerprint plots have been used to examine molecular shapes. The frontier orbital analysis shows that **4** should be more sensitive to a nucleophilic attack than an electrophilic attack. Molecular docking, followed by molecular dynamics simulation and MM-GBSA binding free energy was carried out to predict the binding affinity of **4** for α-amylase enzyme. These analyses revealed good intermolecular stability of the complex with stable high affinity intermolecular complex formation of high equilibrium nature.

1. Introduction

Thiazolidine scaffold compounds exhibit notable medicinal and pharmaceutical properties. In the thiazolidine structure, a major number of replacements are suitable on the 2, 4, and 5 positions for improving the component's medicinal importance. Thiazolidine and thiazolidinone are key components of many natural products and drugs. They exist in many synthetic compounds such as antitumor [1,2], anticancer [3–6], antimicrobial [7–9], anti-diabetic [10], anti-inflammatory [11–13], antiparasitic [14,15], antitubercular [16], antiviral [17, 18], antifungal [19], anti-HIV [20–22], antitrypanosomal [23], cytotoxic [24], antinociceptive and anti-hypernociceptive compounds [25].

Also, thiazolidine derivatives are used as an inhibitor of tyrosyl-DNA phosphodiesterase I [26] and influenza neuraminidase [27], as radioprotective agents against γ-irradiation [28], as pro-drugs for the treatment of cystinosis [29], and as S1P1 receptor agonists [30,31]. They are also used in protein chemical synthesis [32], peptide and protein modification [33], as activators to innate immunity [34] and, also act as immune-stimulating agents [35].

Thiazolidine derivatives participate in several syntheses as potential biomarkers for oxidative stress and formaldehyde exposure [36]. They are also used as synthetic precursors, as heterogeneous catalysts [37,38] and as free radical, superoxide anion radical, and hydroxyl radical scavengers [39–41].

Herein, we report the synthesis and characterization of new 3,3′-ethane-1,2-diylbis(2-benzylidene-1,3-thiazolidin-4-one. Foremostly, an analysis by single-crystal X-ray diffraction has been undertaken to reach a fine description of the architecture of

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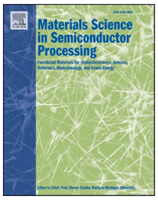

Synthesis, structural and photophysical properties of mixed Zn:SnO_2 nanowires

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ABSTRACT

The present work demonstrates the structural and photophysical properties of mixed zinc tin oxide (Zn:SnO_2) nanowires (NWs) synthesized via vapor transport technique with Zn content of 10, 25 and 50 wt%. The XRD spectra reveals the tetragonal phase of SnO_2 for 10 wt% Zn content, whereas a combination of tetragonal SnO_2 and hexagonal ZnO phases were observed for higher Zn ratios. The SEM images reveals the formation of smooth NWs for low Zn content, whereas a combination of NWs along with spherical nanoparticles have been observed for 50 wt% Zn:SnO_2 sample. The optical band gap was decreased from 3.21 eV (10% Zn:SnO_2) to 2.84 eV (50% Zn:SnO_2), whereas the corresponding Urbach energy increased from 971 meV to 1132 meV. The refractive index values increased from 2.28 to 2.64 when Zn content increased from 10 to 50 wt%. The absorption spectra showed a red shift and the appearance of new band with increasing Zn wt.%, signaling the formation of new electronic states below the conduction band. The fabricated films displayed a broad steady state emission with peak around 462 nm, which intensity decreased with the increasing of Zn ratio. The effective life time of charge carrier was decreased from 198 ps for 10 wt% Zn:SnO_2 to 172 ps for 50 wt% Zn:SnO_2.

1. Introduction

Tin oxide (SnO_2) nanostructures is an excellent semiconducting material characterized by various admirable photophysical properties including high transparency, high mobility, wide band gap ($\sim$ 3.6 eV) and deep energy levels [1]. Moreover, SnO_2 is abundance in nature, environmental friendly, high chemical and mechanical strength and can be synthesized at low temperature [2–6]. Owing to oxygen vacancy and free carries, it can be either n-type or p-type, as well as can be highly reflective in near-infrared (NIR) spectral region. Further, the properties of SnO_2 nanostructures can be easily controlled by varying growth methods and conditions [7–9]. In particular, SnO_2 NWs are characterized by many features such as high surface to volume ratio, high stability and the possibility of syntheses using cost effective methods [10].

These excellent properties led to applications of SnO_2 in various fields such as gas sensors [4,11,12], biosensors [13], catalysis [14], electrode material in energy storage devices [15], photo-thermal shielding coating [16], light emitting diodes [17], etc. Moreover, recently SnO_2 has emerges as alternate of TiO_2 in perovskites solar cells and device based on it have achieved power efficiency in excess of 22% [18]. Although SnO_2 nanostructures show excellent properties but still there is scope to upgrade its optical and electrical properties. Various strategies including UV irradiation [19], metal doping [20], ion-implantation [21], *n-p* heterojunctions [22] have been adopted for optimization and improvement of SnO_2 nanostructure properties.

Metal doping/mixing is the most common strategy used to optimize the properties of SnO_2 nanostructure [23]. However, metal doping of SnO_2 NWs via vapor transport technique is not an easy task. Zinc (Zn) is among the most popular dopants which are used to achieve the improved electron transport properties of SnO_2 nanostructures [7]. The substitution of Sn ions by Zn lead to formation of broken bonds in the structure which act as acceptor energy states above the valance band. These energy states enhance the concentration of holes in valance band by accepting the electrons from there, provides additional paths for the recombination of conduction band electrons through the valance band hole and enhance the luminescence properties [24]. Due to photophysical, chemical and the thermal stability of zinc oxide (ZnO), recent investigations showed the enhanced photocatalytic activities [25,26], sensing properties [26], magnetic properties [27], and photoluminescence [28,29] of mixed Zn:SnO_2 nanostructure.

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Article

Taxonomic Revisiting and Phylogenetic Placement of Two Endangered Plant Species: *Silene leucophylla* Boiss. and *Silene schimperiana* Boiss. (Caryophyllaceae)

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Abstract: The genus *Silene* L. is one of the largest genera in Caryophyllaceae, and is distributed in the Northern Hemisphere and South America. The endemic species *Silene leucophylla* and the near-endemic *S. schimperiana* are native to the Sinai Peninsula, Egypt. They have reduced population size and are endangered on national and international scales. These two species have typically been disregarded in most studies of the genus *Silene*. This research integrates the Scanning Electron Microscope (SEM), species micromorphology, and the phylogenetic analysis of four DNA markers: ITS, *mat*K, *rbc*L and *psb*-A/*trn*-H. Trichomes were observed on the stem of *Silene leucophylla,* while the *S. schimperiana* has a glabrous stem. Irregular epicuticle platelets with sinuate margin were found in *S. schimperiana*. Oblong, bone-shaped, and irregularly arranged epidermal cells were present on the leaf of *S. leucophylla,* while *Silene schimperiana* leaf has "tetra-, penta-, hexa-, and polygonal" epidermal cells. *Silene leucophylla* and *S. schimperiana* have amphistomatic stomata. The Bayesian phylogenetic analysis of each marker individually or in combination represented the first phylogenetic study to reveal the generic and sectional classification of *S. leucophylla* and *S. schimperiana*. Two *Silene* complexes are proposed based on morphological and phylogenetic data. The *Leucophylla* complex was allied to section *Siphonomorpha* and the *Schimperiana* complex was related to section *Sclerocalycinae*. However, these two complexes need further investigation and more exhaustive sampling to infer their complex phylogenetic relationships.

Keywords: endangered; endemic; *Silene*; SEM; stomata; molecular systematics; phylogenetic analysis; nrDNA ITS; cpDNA *matk*; *Siphonomorpha*; *Sclerocalycinae*

1. Introduction

Caryophyllaceae contain 70–86 genera and 2200 species, which are distributed all over the world [1]. The family is divided into four subfamilies: Alsinoideae, Caryophylloideae, Paronychioideae, and Polycarpoideae "Polycarpaoideae" [2]. Within the Caryophylloideae, the tribe Sileneae DC. is regarded as the largest tribe in the family [3].

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Taxonomic Significance of the Leaf Geometric and Micrometric Attributes in the Discrimination of Some Cultivars of *Mangifera indica* L. (Anacardiaceae)

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THE GENUS *Mangifera* L. belongs to the family Anacardiaceae, order Sapindales with 69 known species. *Mangifera indica* is an essential major tropical crop in the globe economy. This study aims to portray the significance of the usage of geometric and micrometric leaf traits to characterize Mango cultivars. Thirty-three morphological and anatomical leaf traits of 41 Mango accessions belong to six cultivars were investigated. The data were analyzed using statistical packages under R environment. Results showed that geometric and micrometric leaf traits such as the leaf length, width, petiole length, leaf blade shape, the shape of upper and lower epidermal cells, the outline of the vascular cylinder, and the number of phloem resin canals were of significance value in the characterization of Mango cultivars. Taxonomic diagnostic key based on some of those traits was constructed. ANOVAs, MANOVA, correlation, and Principal Component Analysis (PCA) retrieved the significance of applying those leaf traits as cultivar identifiers. The present investigation estimate that the attributes of the Mango leaf could be useful and straightforward cultivar identifiers that could be followed by Mango breeders to save time, efforts and money in terms of being unhindered by long juvenile stage of the tree.

Keywords: Juvenile stage, Leaf anatomy, Leaf morphology, Mango, R environment, Taxonomy.

Introduction

The genus *Mangifera* L. belongs to the family Anacardiaceae, order Sapindales (Litz & Hormaza, 2020). Kostermans & Bompard (1993) recognizes 69 species of *Mangifera* based on flower morphology. Most of these are included in two subgenera *Mangifera* L. and Limus (Marchand) Kosterm. The subgenus *Mangifera* contains most of the species (47) distributed into four sections: section Marchandora Pierre.; section Euantherae Pierre.; section Rawa Kosterm.; and section *Mangifera* Ding Hou. A further 11 species reside in uncertain classification positions (Kostermans & Bompard, 1993). The origin and the center of *Mangifera* diversity has been established as South-East Asia and, from here it has spread and is now cultivated across the world (Bompard, 2009). According to Abdelsalam et al. (2018) *Mangifera indica* L. (Mango), was introduced for cultivation in Egypt at least 200 years ago. In 2015, the total cultivated area of Mango reached ~ 102071.76 hectares, with the main cultivation area concentrated in the Ismailia Governorate.

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Article

The devastating flood in the arid region a consequence of rainfall and dam failure: Case study, Al-Lith flood on 23th November 2018, Kingdom of Saudi Arabia

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With 11 figures and 6 tables

Abstract: On November 23, 2018, cascading rainfall events that occurred in the upstream section of wadi Al-Lith, which is located in the western part of the Kingdom of Saudi Arabia, caused a failure in the Al-Lith earthen dam. This event was followed by a large-scale devastating flood that inundated the area downstream of the dam, damaging infrastructure and property. The main scope of this work was to identify the causes of catastrophic flooding and ways to prevent and mitigate the potential consequences of a future flood occurrence in the study area. For this purpose, remote sensing images, DEM, field observations, and rainfall data were used. A geospatial integrated approach using a GIS, remote sensing, hydromorphological analysis, and rainfall-runoff modeling was utilized to provide a better understanding of the hydrology of the wadi Al-Lith catchment. Various methods were used for rainfall frequency analyses; supervised classification was applied on Landsat (OLI), in which land-use types were classified to identify the curve number values. Rainfall-runoff modeling was conducted using the catchment characteristics and rainfall analysis to calculate flood volumes and peak discharges. Peak discharge results at the flood event on November 23, 2018, and at 5- and 100-year return periods were used for the prediction of flood extent using the 2D HEC-RAS model. Water inundated depth and velocity were mapped. The result of the 5-year return period simulated model showed a good correlation with the flood extent of the event on November 23, 2018 that extracted from the sentinel-2 image. This model was validated using field observation data and remote sensing interpretation at the real flood event of November 2018. The flood model indicated that a dam failure with the substantial release of an enormous amount of water in a short period created exacerbates the problem. Also, the simulated model of the 100-year return period showed high-risk of the whole floodplain area of Wadi Al-Lith and the urbanized zone, where utterly devastation could be occurred. Finally, the results showed that a new dam proposal is urgently required to prevent the area from future flood events to replace the failed dam with a 45 m high dam. In this case, the reservoir capacity is estimated to be ~147.4 million m^3, which is above the runoff volume for a 200-year return period.

Keywords: devastating floods; dam failure; inundation; Al-Lith; Kingdom of Saudi Arabia

1 Introduction

Flash floods in arid areas are often characterized by high intensity and short duration, which, when combined with the minimal response time due to fast water runoff and lack of adequate warning systems, leads to an increase in the risk to human lives and property (Karymbalis et al. 2011, Moawad 2016, Sene 2013, Youssef et al. 2016). Extreme rainfall events are considered a crucial triggering factor causing floods and landslides, which are the

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The Digital Transformation Effects in Distance Education in Light of the Epidemics (COVID-19) in Egypt

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Abstract:

On the relatively rare occasions when disaster forces schools and universities to close for a prolonged period of time, e-learning has helped fill the gap in instruction. In this paper, we study the role of digital transformation in e-learning systems in light of the global conditions resulting from the epidemics (COVID-19) in Egypt. Therefore, we focus on the importance of distance education at several factors, trying to assess the staff's response and students to new education methods and assess the distance education experience in Egyptian universities. Where the study set that various staff excited to utilize this method, unlike some of the students, who did not to accept because of their knowledge lacking.

Keywords: Distance Education, COVID-19, Digital transformation.

1 Introduction

Humanity knew the end of the twentieth century, and the beginning of the twenty-first as a huge revolution in the field of modern information and communication technology, which leads to a different world in terms of data, tools, text, voice, and image being transferred and dealt with via the Internet world, which creates a new world through which it can form educational environments and promote creativity in it [1]. Which made the current era characterized by amazing developments in information and communications technology field, which contributed to establishing new milestones. Modern information systems in the digital age shadow are analytical and diagnostic systems, that give broad capabilities for flexible and effective analysis, planning, and effective response to the changes surrounding the work environment. The changes are taking place in the work environment and qualify them to be more able to create and invest opportunities [2]. Educational institutions do not live alone from these global variables, especially higher education institutions where the future of universities today is related to these rapid developments in the field of knowledge and technology and the accompanying infinite flow of visions, trends, goals and ideologies, the reality and nature of the challenges facing universities imposed many important transformations in University education systems, so any development depends on the university's ability to realize the importance of change and monitor its impacts in long and short term, and this requires the formation of highly qualified human resources as an important component of survival in the digital age[3], so it has become imperative for it. A striving to participate in making this future and defining its roles in preparing human wealth and building individuals with competence and excellence to deal with the challenges of the third millennium [4].

Since the launch of the distance education [5, 6] program, many difficulties and obstacles that may face its spread and effectiveness have started to appear: Are all students equipped with enough electronic devices (computers, tablets, smartphones) to rely on them in distance education? Do all students have a sufficiently strong internet connection that enables them to access and benefit from the lessons and programs broadcast on digital distance education channels? Do all students in villages and remote areas have access to strong internet coverage and before we talk about it, do you already own these digital devices? Has a technological infrastructure been provided

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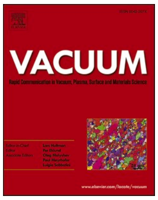

The effective reduction of graphene oxide films using RF oxygen plasma treatment

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Graphene oxide (GO)
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ABSTRACT

Graphene Oxide (GO) has attracted strong research interest due to its unique mechanical, thermal, electrical, and magnetic properties. Herein, a simple oxygen plasma process is used as an eco-friendly, novel and effective surface treatment technique to enhance the microstructure, adhesion force, and electrical properties of the GO films. GO films were treated in a plasma oxygen environment at a constant RF power of 300 W and different processing times ranging from 0 to 7 min. X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy are utilized to examine changes in the type of surface groups and the distribution of bonds energy before and after plasma treatment. Additionally, the effect of RF oxygen plasma treatment on other properties, such as thermal stability, surface roughness, contact angle, work of adhesion, wettability, electrical conductivity, and sheet resistance has been studied. XPS data revealed that RF oxygen plasma treatment reduced the amount of oxygen-containing groups (such as epoxides (O–C═O), carbonyls (C–O–C), and carboxyl's (O–C═O) from 48.8% for the as-prepared GO film to 33.56% after 5 min of treatment. In addition, the average surface roughness (Ra) increased from ~7.8 of as-prepared GO film to ~8.7 μm, while the work of adhesion improved to reach 134.84 mN/m. However, with increasing plasma processing time up to 7 min, the thermogravimetric analysis (TGA) of the treated GO film showed a weight loss difference of 51.66%. Furthermore, introducing a high amount of C═O bonds (carbonyl and SP^2 groups of carbon atoms) after plasma treatment improved the electrical conductivity to a value of 0.156 S/m. The current results indicate that the properties of GO can be tuned by varying the degree of oxidation, which may pave the way for new developments in GO-based applications.

1. Introduction

Graphene is a monolayer of carbon atoms detached from inexpensive pure graphite that is packed into 2-D honeycomb lattices [1]. Graphene oxide (GO) is an oxygenated derivative of graphene. It has abundant functional groups of oxygen and can be exfoliated and dispersed easily in different solvents including water [2,3]. Graphene and its derivatives have enormous expectations for usage in many applications, while its low electrical conductivity is still a challenging problem. Therefore, reducing the GO sheets is considered as one of the effective ways to enhance its electrical properties. The reduced graphene oxide (rGO) has a wider range of applications than GO or even pure graphene, such as an electrode for Li-ion batteries [4], photoconductive switching [5], catalyst [6], supercapacitors [7], sensors [8], biological imaging [9], etc. As known, GO can be chemically or thermally reduced to obtain graphene-like properties. Annealing of GO at high temperatures has used as a thermal reduction technique [10]. Likewise, the chemical reduction can be obtained using strong reducing chemicals, such as hydrazine (N_2H_4) [11] and borohydride ($NaBH_4$) [12]. At the same time, these reducing chemical substances are dangerous and environmental pollutants. It has been found that the rGO sheets produced by chemical or thermal reduction have more defects and poor conductivity, which reduces the carrier mobility restricting its usage in the electronic applications [13]. Alternatively, reduction by radio-frequency (RF) plasma discharge is considered as a more effective, safe, rapid reduction technique as well as an environmentally-friendly method, compared to other chemical and thermal techniques [14]. The RF plasma can be generated using a radio-frequency electric field of 13.56 MHz. In this process, with

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ORIGINAL PAPER

The impact of indium metal as a minor bimetal on the anodic dissolution and passivation performance of zinc for alkaline batteries. Part II: galvanostatic, impedance spectroscopy, and charge–discharge evaluations

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Abstract

The anodic dissolution and passivation processes of zinc and zinc-indium alloys were investigated in an alkaline solution of 6 M KOH using galvanostatic, electrochemical impedance, and charge–discharge measurements. Galvanostatic measurements exhibit anodic potential/time transient of the zinc anode and its alloys in the concentrated alkaline solution at different current densities. The data reveal that the passivation time ($t_{pass.}$) diminishes with increasing the content of indium in the alloy under investigation. This means that the alloying of minor indium with zinc retards its dissolution at the active region. The high oscillations in potential, which are observed in the case of zinc, disappeared with the addition of a minor indium content to zinc (Zn-In alloy). The data acquired from impedance (EIS) exhibited that the values of polarization resistance (R_p) and Warburg impedance increase, while the double-layer capacitance (C_{dl}) diminishes with increasing a minor indium content at both two investigated potentials (−500 and + 500 mV vs. SCE). It is interesting to show that the inductive loop for alloys I and II at −500 mV is observed at intermediate frequencies, in addition to the capacitive loop and Warburg tail. The results of charge–discharge measurements show that the average charge–discharge separation voltages of alloys I and II are 0.8 and 0.9 V, respectively, which are higher than that of pure zinc (0.7 V) at constant time. This indicates that indium alloying with zinc leads to improvement in both energy and charge efficiency.

Keywords Zn-in alloys · Galvanostatic measurements · Impedance · Charge–discharge properties · Charge efficiency · Specific capacitance

Introduction

As the demand for energy increases in modern societies, both energy crises and environmental deterioration have encouraged the development of high-performance devices based on energy storage with non-toxic, ecologically friendly, relatively low-cost peculiarities. In energy storage research, much attention has been paid to metal-air batteries, which are considered an attractive alternative energy source for the future. Nowadays, rechargeable batteries based on metal-air have attracted global attention [1–3]. Zinc is used as an anode material in both alkaline and chloride batteries, due to its electrochemical and environmental characteristics [4]. But, alkaline batteries are predominantly used as an efficient energy source in many electronic devices. However, zinc is highly corroded in alkaline solution, owing to its high activity [5], and this behavior remains a difficult problem. Therefore, the electrochemical and corrosion manner of zinc anode has attracted the interest of many studies in alkaline media [6–12]. The previous works showed that the dissolution process of zinc in an alkaline solution is the main cause for the appearance of oxide and hydroxide layer on its surface [11]. Besides, the zinc electrode in an alkaline battery has disadvantages during the operation such as dendritic formation through cycles, passivation of the surface, and evolution of hydrogen gas [13]. Through the charge–discharge process, the dendrite structure progressively generates and leading to a diminishing in the electrochemical

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The joint adverse effects of aged nanoscale plastic debris and their co-occurring benzo[α]pyrene in freshwater mussel (*Anodonta anatina*)

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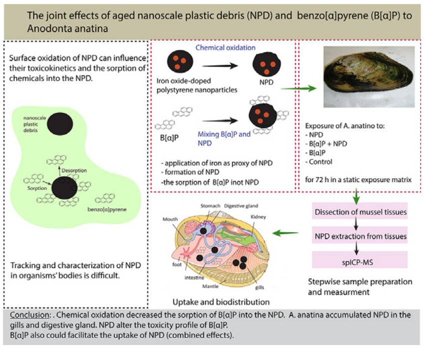
HIGHLIGHTS

- Chemical oxidation decreased the sorption of B[α]P into nanoscale plastic debris (NPD).
- After 72-h of exposure, *A. anatina* accumulated NPD in gills and digestive gland.
- Presence of B[α]P increases accumulation of NPD in the tissues of mussels.
- The mixture of NPD and B[α]P increased the activity of SOD and CAT enzymes.

GRAPHICAL ABSTRACT


The joint effects of aged nanoscale plastic debris (NPD) and benzo[α]pyrene (B[α]P) to Anodonta anatina

Surface oxidation of NPD can influence their toxicokinetics and the sorption of chemicals into the NPD.

Tracking and characterization of NPD in organisms' bodies is difficult.

- application of iron as proxy of NPD
- formation of NPD
-the sorption of B[α]P inot NPD

Exposure of A. anatino to:
- NPD
- B[α]P + NPD
- B[α]P
- Control

for 72 h in a static exposure matrix

Stepwise sample preparation and measurment

Conclusion: . Chemical oxidation decreased the sorption of B[α]P into the NPD. A. anatina accumulated NPD in the gills and digestive gland. NPD alter the toxicity profile of B[α]P.
B[α]P also could facilitate the uptake of NPD (combined effects).

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ABSTRACT

Although the presence of small-scale plastics, including nanoscale plastic debris (NPD, size <1 μm), is expected in the environment, our understanding of their potential uptake and biodistribution in organisms is still limited. This mostly is because of the limitations in analytical techniques to characterize NPD in organisms' bodies. Moreover, it is still debatable whether aged NPD can sorb and transfer chemicals into organisms. Here, we apply iron oxide-doped polystyrene nanoparticles (Fe-PS NPs) of 270 nm size to quantify the uptake and biodistribution of NPD in freshwater mussels (*Anodonta anatina*). The Fe-PS NPs were, first, oxidized using heat-activated potassium persulfate treatments to produce NPD (aged particles). Then, the sorption of benzo[*a*]pyrene (B[α]P), as a model of organic chemicals, into the aged NPD was studied. Chemical oxidation (i.e. aging) significantly decreased the sorption of B[α]P into the particles over 5 days when compared to pristine particles. After 72-h of exposure, *A. anatina* accumulated NPD in the gills and digestive gland. When exposed to the mixture of NPD and B[α]P, the number of particles in the gills and digestive gland increased significantly compared to the mussels exposed to NPD alone. Moreover, the mixture of NPD and B[α]P increased the activity of Superoxide dismutase and Catalase enzymes in the exposed mussels when compared to the control and to the NPD alone. The present study provides evidence that aged NPD not only could accumulate and alter the toxicity profile of organic chemicals in aquatic organisms, but the chemicals also could facilitate the uptake of NPD (combined effects).

1. Introduction

Large plastic debris in the environment gradually degrades into smaller pieces because of weathering, including ultraviolet radiation,

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RESEARCH ARTICLE

The protective role of lycopene against toxic effects induced by the herbicide Harness® and its active ingredient acetochlor on the African catfish *Clarias gariepinus* (Burchell, 1822)

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Abstract

The effects of Harness® toxicity on fish health are little known. So, current work aimed to study the impact of sub-lethal doses of Harness® (an acetochlor-based herbicide) on the African catfish, *Clarias gariepinus*, and also investigated the potential role of lycopene (LYCO) administration in alleviating Harness® negative effects. Fish were divided into five groups in triplicates as follows: group 1 (control) received no treatment, group 2 was exposed to 10 μm Harness®/L, group 3 was orally administered 10 mg LYCO/kg body weight and exposed to 10 μm Harness®/L, group 4 was exposed to 100 μm Harness®/L, and group 5 was orally administered 10 mg LYCO/kg body weight and exposed to 100 μm Harness®/L for 2 weeks. Some hemato-biochemical parameters, genotoxicity, and histopathological changes were assessed at the end of this period. Sub-lethal doses of Harness® altered the shape of erythrocytes in contrast to the control sample. Also, hematological parameters of exposed fish exhibited a significant ($P < 0.05$) reduction in the values of red blood cell count (RBCs), hemoglobin (Hb), hematocrit (HCT), and platelets (PL), as well as an insignificant ($P > 0.05$) drop in mean corpuscular volume (MCV). Harness® was also found to cause genotoxicity as well as histopathological alterations. LYCO administration decreased hemato-biochemical changes and returned them to near-normal levels. The findings showed that LYCO administration (10 mg LYCO/kg body weight) decreased Harness® toxicity in *C. gariepinus* and alleviated its destructive effects.

Keywords Harness® · Acetochlor · Lycopene · *Clarias gariepinus* · Hematology · Biochemical

Introduction

Water contamination has been one of the world's most critical issues in recent decades. The primary cause of water body depletion in many developed countries is the massive pace of rising industries, urbanization, agricultural and domestic sanitation, and numerous human activities (Arif et al. 2020; Haredi et al. 2020). Polluted water reduces the consistency of water sources and harms aquatic species (Fatima et al. 2020).

Herbicides' ubiquitous, persistent, and substantial use of agricultural processes have resulted in pollution of nearby water sources, posing a danger to various aquatic biota, including fish (Guo et al. 2008). Harness® is a commercial herbicide that contains acetochlor (ACET) at a concentration of 84% as an active ingredient. ACET is the common name for 2′-chloro-N-(ethoxymethyl)-N-(2-ethyl-6′-methylphenyl) acetamide [CAS number 34256-82-1] (Heydens et al. 2010). It is a selective, systemic pre- and post-emergence chloroacetamide herbicide commonly used in crops to combat annual grasses and broadleaf weeds (Liu et al. 2020). It is certified for various crops and over forty countries worldwide (Guo et al. 2020; Hoogeweg et al. 2020). According to the United States Environmental Protection Agency (USEPA), it is the third most widely used herbicide in the global agricultural market (Chang et al. 2020). In water environments, ACET has low sorption, high stability,

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Theoretical analysis of the effect of doping and minority charge carrier life time in CIGS solar cells

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In this work the optical and recombination losses for CuInGaSe (*CIGS*) thin-film solar cells have been theoretically studied. The optical losses have been studied on the basis of the thickness of frontal charge-collecting layer (*ZnO:Al*) effect. The recombination losses have been studied as a function of *CIGS* doping (N_A) and electron lifetime (τ_n). The optical and recombination losses effect on short circuit current density, (J_{sc}), the open circuit voltage (V_{oc}), the fill factor (*FF*) and conversion efficiency (η) of thin-film solar cells based on *n*-CdS/*p-CIGS* has been investigated. It was found that the film with the transparent conducting layer 100 nm thickness is suitable to give the highest J_{sc} value of about 29.5 mA/cm^2 and the lowest value of optical losses of about 26%. The *CIGS* doping has a significant effect on the values and behavior of the internal efficiency. There is a weak effect of the relaxation time on the efficiency of this solar cell as it increases from 18.7% to 19.1% with increase the lifetime from the value of 10 nS to 80 nS, respectively.

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Keywords: CIGS, Solar cell, Optical loss, Recombination loss and the efficiency

1. Introduction

Cu(In, Ga)Se$_2$ *(CIGS)* is considered one of the most promising second generation solar cells based on thin- film technologies with highest efficiencies which confirmed in the world. Tiwari group (EMPA Switzerland) reported recently a record efficiency of 20.4% on flexible polymer foil (23% in glass) [1]. The value 21.7% is the most recent record efficiency obtained in a laboratory environment [2-4]. There are large- area terrestrial applications of *CIGS* potential advantages, in addition *CIGS* photovoltaic can be made very lightweight and flexible which is desirable for building integrated and portable applications and have also shown high radiation resistance, compared to crystalline silicon and III-V cells so they are also promising for space applications [5, 6]. Many studied have concerned the optical, electrical and structural properties of each layer of thin-film solar cell such as the transparent conducting layer, n-type layer and the absorber layer [7-9]. Along with the experimental works, the solar cell modelling [10-15] has become indispensable tool used to analyse the performance and optimizing the design of any kind of efficient solar cells.

In this work, Mohamed model [16-19] have been used to study the effect of doping and electron lifetime on the *CIGS* solar cell performance. In this article the optical and recombination losses have been considered in *CIGS* devices, as it is important causes of low solar to electric energy conversion. The quantitative estimation of the optical losses has been carried out based on the optical constants of the used materials. On the other hand, the recombination losses at the front and the back surface of the absorber layer have been determined by using the continuity equation taking into account the drift and diffusion components of the photocurrent.

2. The simulation details

In this model, the absorber *CIGS* is a p- type, with different doping, the junction is made between the *CIGS* and n-type *CdS* which has a gap of 2.45 eV. The window layer is formed from *ZnO:Al* ceramic (ZnO 98 wt%, Al$_2$O$_3$ 2 wt%) with a gap equals to 3.3 eV [20]. The data of CIGS were taken from Refs. [14, 21], where CIGS films were deposited by simultaneous thermal evaporation of elemental copper, indium, gallium and selenium. In this study, the spectrum was set to the global AM 1.5 standard and the operation temperature was maintained at 300 K. Through this model, the optical losses result from the reflection at air/*ZnO:Al, ZnO:Al*/*CdS, CdS*/*CIGS* interfaces and the light absorption in *ZnO:Al* and *CdS* layers as well as the recombination losses at the front and back surface of *CIGS* can be quantitatively assessment. The quantitative estimation of the optical losses is carried out passed on the refractive index, extinction coefficient and the optical band gap of the used materials. The recombination losses determined by employ the continuity equation that taking into account the drift and diffusion components of the photocurrent. The quantitative determination of the recombination losses is carried out based on the physical properties of the absorber layer (*CIGS*) such as; the absorption coefficient, energy band gap, thickness, carrier lifetime, mobility, etc. This study concerns on the effect of *CIGS* doping (N_A) and carrier life time (τ_n) on the solar cell efficiency.

2.1. CIGS solar cells structure

The schematic structure of substrate thin- film solar cell based on *CIGS* is shown in Fig. 1. The configuration of the *CIGS* layer can differ between different *CIGS* solar

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Thermal and Electrical Properties of $(CdS)_{1-x}$ $(ZnS)_x$ Thin-Films Deposited by Thermal Evaporation Technique

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Abstract: Thin-films of CdS doped with various ZnS contents have been deposited using thermal evaporation technique. The thermal and electrical properties of the deposited films have been studied. The DC electrical conductivity of $(CdS)_{1-x}(ZnS)_x$ thin films were calculated from the resistance measurements using two-probe method. It was found that the Seebeck coefficient (*S*) of $(CdS)_{1-x}(ZnS)_x$ thin films measured at room temperature has a negative sign indicating that $(CdS)_{1-x}(ZnS)_x$ thin films were n-type semiconductors for different ZnS contents. The values of *S* found to increase with increasing ZnS content. Also, the conductivity decreased from 1646 $(\Omega.cm)^{-1}$ to 818 $(\Omega.cm)^{-1}$ with increasing ZnS content from x=0 to 0.5, respectively. Some important parameters such as the mean free bath, carrier concentration, carrier mobility, diffusion coefficient, Fermi energy and effective mass were calculated from the thermal and electrical measurements.

Keywords: CdS – CdS – Thin-Films – Electrical Properties – Thermal Properties.

1 Introduction

For the last decade, Cadmium Sulfide (CdS) thin film has attracted increased attention because of its wide direct optical band gap, good optical and electrical properties, high electron affinity, stability and n-type conductivity [1, 2]. CdS thin film is applied as a window material and as a heterojunction partner in thin films based on heterojunction solar cells such as CdTe [3], $CuInS_2$ [4], $CuInGaS_2$ [5], $Cu_2ZnSn(S,Se)_4$ [6] and PbS [7].

The optical band gap of CdS is relatively low (2.42 eV), hence the photons with energy higher than 2.42 eV may be absorbed by CdS layer before reaching the absorber layer. There are three ways to solve this problem: first is to reduce the CdS layer thickness, second is to substitute CdS by a wide optical band gap semiconductor like ZnS [8] and third is to increase the optical band gap of CdS. Reducing the thickness of CdS may be lead directly to increase the short-circuit current density. However, the thickness must not too thin to avoid short circuit effects due to forming the pinholes [9]. On the other hand, reducing the thickness usually severely reduces the open circuit voltage and fill factor [10].

The process of doping CdS with a wider optical band gap semiconductor such as ZnS may be the best solution to improve the optical and electrical properties of CdS in order to use it as a window layer in thin-film solar cells. In this aspect, the doping type, the ratio of doping and the type of deposition techniques are considered most important factors in this process.

CdS thin films have been prepared by diverse techniques including chemical bath deposition [11], electrodeposition [12], laser ablation [13], sputtering [14], vacuum evaporation [15] etc. Thermal evaporation method is the most commonly method for constructing amorphous solid in the form of thin film due to its simplicity. The materials that are deposited by evaporation include metals, semiconductors, alloys, mixtures thereof, refractory compounds (i.e. oxides, carbides, nitrites, borides, etc.) and intermetallic compounds

In this work, thin- films of CdS doped with various ZnS contents have been prepared by a thermal evaporation technique. The effect of ZnS-content on thermoelectric

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Research Article

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Thraustochytrids from the Red Sea mangroves in Saudi Arabia and their abilities to produce docosahexaenoic acid

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Abstract: This is the first study of thraustochytrids from the Red Sea coast in Saudi Arabia. One hundred and thirty-four isolates of thraustochytids were cultured from Al-Leith, Jeddah and Yanbu mangroves from this area, and were categorized into 38 morphotypes. Among the isolated thraustochytrids, *Aurantiochytrium* was the most speciose genus, represented by 36 morphological types. Seventeen strains formed a distinct clade within the genus *Aurantiochytrium* based on phylogenetic analyses of 18S rDNA sequences. The *Aurantiochytrium* clade from the Middle East is characterized by the production of high levels of oleic and linoleic acids and may represent undescribed taxa. Four *Aurantiochytrium* strains were grown on large scale to study their ability to produce docosahexaenoic acid (DHA). These strains produced biomass ranging from 37.7 to 66 g L^{-1} and the percentages of oil ranged from 40 to 57.2% of the dry weight. Twenty-one fatty acids were recorded from the four strains which included: eight saturated four mono-unsaturated and nine polyunsaturated. Dominant fatty acids included C16:0 palmitic acid (24.14–37.02% total fatty acid (TFA)), C18:1ω9 oleic acid (3.01–25.07% TFA), C18:2ω6 linoleic acid (1.85–20.85% TFA) and C22:6ω3 DHA (4.87–16.5% TFA). DHA was the predominant polyunsaturated fatty acid in three strains, while linoleic acid was the predominant PUFAs in one strain.

Keywords: *Aurantiochytrium*; heterokonta; molecular phylogenetics; PUFA; straminopiles–subtropical microbes.

1 Introduction

Thraustochytrids are a group of unicellular heterotrophic protists that are ubiquitous in their distribution within marine environments (e.g. Bahnweg and Sparrow 1974; Ganuza et al. 2019; Lee Chang et al. 2012; Lewis et al. 1998; Lyu et al. 2021; Manikan et al. 2015; Marchan et al. 2018; Naganuma et al. 1998; Raghukumar and Gaertner 1980). Thraustochytrids belong to the class Labyrinthulea, and are characterized by their heterokont, biflagellate zoospores closely related to heterokont algae (Kingdom: Chromista) (Cavalier-Smith et al. 1994; Cavalier-Smith and Chao 2005; Lewis et al. 1999). Thraustochytrids can ferment a wide range of substrates to produce value-added products (e.g. omega-3 polyunsaturated fatty acids (PUFAs), biodiesel feedstocks, squalene and carotenoids), that have wide applications in neutraceutical and cosmetic industries (Chen et al. 2015, 2020). Moreover, biomass of thraustochytrids can be used as feed for marine fish and poultry to improve the quality of the animals' products (Burja et al. 2006; Singh et al. 2014; Ueda et al. 2015).

Sparrow (1936) described the first thraustochytrid species and placed it within the fungi because of their heterotrophic nature and superficial resemblance to euchytrids. In the following three decades several species were described from various marine habitats (Goldstein 1963; Sparrow 1943; Vishniac 1956) and by the 1990s, their physiological requirements had been extensively studied (Bahnweg 1979; Bremer 1976; Gaertner 1979; Jones and Harrison 1976; Moss 1986; Perkins 1973; Porter 1986; Ulken et al. 1985). Since the

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SURFACE and INTERFACE ANALYSIS WILEY

RESEARCH ARTICLE

Time-of-flight secondary ion mass spectrometry and gas chromatography–mass spectrometry studies of alkanethiol self-assembled monolayers on nanoporous gold surfaces

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The dimerization of alkanethiol mixtures (hexanethiol, octanethiol, and dodecanethiol) to form self-assembled monolayers (SAMs) from headspace on nanoporous gold surfaces was studied for the first time using gas chromatography (GC/MS) and time-of-flight secondary ion mass spectrometry (TOF-SIMS). The nanoporous gold surfaces were obtained by an acidic etching of a 585-gold alloy. Field emission scanning electron microscopy (FE-SEM) was utilized to study the change of the surface geometry and porosity of the gold surfaces before and after etching. Alkanethiols were deposited from the vapor phase above the thiol solutions (headspace) on nanoporous gold plates and nanoporous gold solid-phase vmicroextraction (SPME) fibers. The nanoporous gold substrates were analyzed by TOF-SIMS and GC/MS, respectively. The TOF-SIMS spectra exhibited various gold–sulfur ion clusters and specific peaks related to the adsorption of thiols such as deprotonated monomers, thiolate–Au, dimers (e.g., dialkyl sulfides–Au and dialkyl disulfides–Au). The GC/MS analysis of headspace extractions of alkanethiol mixtures by nanoporous gold SPME fibers showed a high extraction efficiency of alkanethiol, dialkyl sulfide, and dialkyl disulfide when compared with the commercial SPME fibers (DVB-CAR-PDMS and CAR-PDMS). Different GC/MS optimization factors were studied including the extraction time and desorption temperature.

KEYWORDS
dimerization of SAMs, GC/MS, nanoporous gold, solid-phase microextraction (SPME), TOF-SIMS

1 | INTRODUCTION

Nanoporous gold has been widely used in different applications and industrial areas such as catalysis, separations, fuel cells, sensors, and biomedical applications.[1–5] Because of its high surface porosity, stability, and good conductivity, nanoporous gold is used in different research areas of analytical chemistry.[6–10] According to the different activities of various metals in a gold alloy, one or more metals could dissolve during an acidic etching of the alloy to obtain a uniform structure nanoporous gold surface with a high specific surface area. Such a dealloying method is convenient and easy to operate.[7,10]

Self-assembled monolayers (SAMs) of alkanethiols and their derivatives on gold surfaces have been of great interest for many decades because of the high affinity between gold substrates and the sulfur head group in alkanethiols. Alkanethiolate SAMs on gold surfaces are generally stable in an environment with an absence of air for a couple of days,[11–17] so they can be characterized by many analytical techniques such as scanning tunneling microscopy,[12] atomic force microscopy,[13] x-ray photoelectron spectroscopy (XPS),[14] and time-of-flight secondary ion mass spectrometry (TOF-SIMS).[7,15] TOF-SIMS is a powerful technique for surface characterization in static and dynamic modes of analysis.[18] SIMS shows also good feasibility in the

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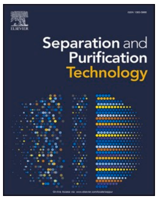

TiO_2-carbon microspheres as photocatalysts for effective remediation of pharmaceuticals under simulated solar light

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ABSTRACT

In this work, novel carbon microspheres supported TiO_2 nanoparticles were prepared for the degradation of pharmaceuticals in water, selecting diclofenac, acetaminophen, and ibuprofen as target pollutants. Lignin, an important biomass byproduct from the paper industry and biorefineries, was transformed in carbon microspheres by a novel approach based on a Fe-activated hydrothermal carbonization followed by pyrolysis at 900 °C. These carbon microspheres were further covered with TiO_2 by a solvothermal treatment. The effects of several parameters including hydrothermal carbonization time and mass ratio (TiO_2:carbon) on the catalytic activity of TiO_2-carbon microspheres were investigated. The results revealed that the combination of long carbonization time and high TiO_2:carbon ratio achieved superior TiO_2-carbon microspheres (Ti2-C20) catalytic performance. Ti2-C20 achieved complete degradation of ibuprofen (5 $mg\cdot L^{-1}$) and diclofenac (5 $mg\cdot L^{-1}$) within 3 h under solar light and mineralization percentages close to 50%. Moreover, the photocatalytic performance remained high after five reuse cycles and was barely affected by the presence of common inorganic ions in treated wastewater (such as Cl^-, NO_3^- and HCO_3^-). The degradation pathway of diclofenac was proposed, involving C-N bond cleavage, and subsequent hydroxylation and cyclization reactions leading to the formation of aliphatic carboxylic acids. Overall, promising photocatalysts were obtained from a biomass byproduct for effective degradation of pharmaceuticals with the assistance of solar light.

1. Introduction

The presence of pharmaceutical residues in wastewater effluents poses an environmental threat due to their adverse biological activity, affecting their likely reuse (as treated wastewater or “reclaimed” water). Analgesic and anti-inflammatory drugs (e.g., diclofenac, DCF; ibuprofen, IBU; and acetaminophen, ACE) are among the most common commercially distributed pharmaceuticals. They are frequently detected in those effluents at concentration levels above the ecotoxicity endpoints of different organisms (i.e., from a few $ng\cdot L^{-1}$ to several $mg\cdot L^{-1}$) [1,2]. Conventional treatment technologies used at wastewater treatment plants (WWTPS) can only achieve partial removal (~21–40%) of these compounds [3]. Stimulated by these facts, several treatment methods have been investigated for the removal of pharmaceuticals in water [4]. Among them, advanced oxidation processes (AOPs) proved to be very efficient in the degradation of these contaminants. Solar-driven photocatalysis has gained increasing interest as environmentally friendly and cost-effective potential solution for the abatement of emerging contaminants, including pharmaceuticals and personal care products [5,6].

Titanium dioxide (TiO_2) is the most used semiconductor in photocatalysis due to its established activity and relatively low toxicity compared to other types of photocatalysts [7]. However, the application of TiO_2 nanoparticles in slurry configuration makes the recovery of the photocatalyst difficult [8]. Although anchoring the semiconductor on a support may introduce mass transfer limitations, it is expected to facilitate the postseparation process of the photocatalyst [9–11]. In this respect, carbon spheres have gained increasing interest as supports due to their high structural stability, tunable porosity and particle size [12,13]. The extensive research performed by Titirici et al. [14–16] revealed some of these promising advantages and likely applications

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Structural, conformational and therapeutic studies on new thiazole complexes: drug-likeness and MOE-simulation assessments

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Abstract

A series of new complexes derived from Pd(II), Cu(II) and Fe(III) ions reacted with thiazole derivative (HL, CPTP) was prepared. Structures of all new compounds were characterized and confirmed using analytical and spectroscopic (IR, UV–Vis and ^{13}C&^{1}H NMR) techniques. All complexes have non-electrolytic nature based on molar conductance measurements. TGA was executed to confirm the presence of water molecules inside or outside the coordination sphere as well as the mono-nuclear feature of isolated complexes. Accordingly, thermo kinetic parameters were calculated for all decomposition steps. The obtained analytical data regarding complexation in solution, molar ratio and continuous variation methods suggest 1 M:1 L molar ratio. The oriented structures using advanced program assert on best distribution for coordinating sites (NH& NH_2). Moreover, electrostatic potential map as well as iso-surface with array plot of ligand reflects high nucleophilic feature with reduced outer contour on two coordinating sites. In vitro antimicrobial, anticancer and antioxidant activities of ligand and its complexes were checked. All complexes exhibited superiority on free ligand in successful treatment, specifically CPTPPd complex. Drug-likeness as well as MOE-docking simulation outcomes indicates promising inhibitory feature of CPTPPd and CPTPCu complexes, in agreement with in vitro results.

Supplementary information The online version of this article (https://doi.org/10.1007/s11164-020-04380-9) contains supplementary material, which is available to authorized users.

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Article

Development of New Thiazole Complexes as Powerful Catalysts for Synthesis of Pyrazole-4-Carbonitrile Derivatives under Ultrasonic Irradiation Condition Supported by DFT Studies

Mahmoud Abd El Aleem Ali Ali El-Remaily,* Tarek El-Dabea, Mohammed Alsawat, Mohamed H. H. Mahmoud, Alia Abdulaziz Alfi, Nashwa El-Metwaly,* and Ahmed M. Abu-Dief*

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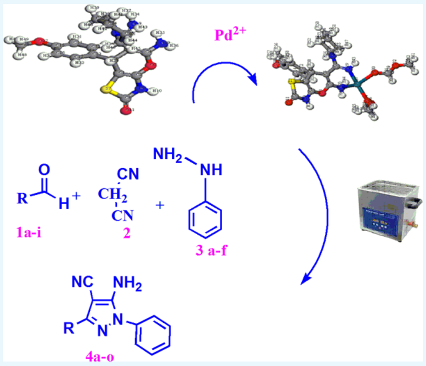
ABSTRACT: In this study, we are interested in preparing Fe(III), Pd(II), and Cu(II) complexes from new thiazole derivatives. All syntheses were elaborately elucidated to estimate their molecular and structural formulae, which agreed with those of mononuclear complexes. The square-planer geometry of Pd(II) complex (MATYPd) was the starting point for its use as a heterocatalyst in preparing pyrazole-4-carbonitrile derivatives **4a−o** using ultrasonic irradiation through a facile one-pot reaction. The simple operation, short-time reaction (20 min), and high efficiency (97%) were the special advantages of this protocol. Furthermore, this green synthesis strategy was advanced by examination of the reusability of the catalyst in four consecutive cycles without significant loss of catalytic activity. The new synthesis strategy presented remarkable advantages in terms of safety, simplicity, stability, mild conditions, short reaction time, excellent yields, and use of a H_2O solvent. This catalytic protocol was confirmed by the density functional theory (DFT) study, which reflected the specific characteristics of such a complex. Logical mechanisms have been suggested for the successfully exerted essential physical parameters that confirmed the superiority of the Pd(II) complex in the catalytic role. Optical band gap, electrophilicity, and electronegativity features, which are essential parameters for the catalytic behavior of the Pd(II) complex, are based mainly on the unsaturated valence shell of Pd(II).



1. INTRODUCTION

Heterocyclic compounds of pyrazoles class are known by their importance in pharmaceutical targets and medicinal interest. Organic derivatives enriched by S and/or N atoms have a broad spectrum of biological activities such as antimicrobial, antioxidant,[1,2] anti-HIV, anticancer,[3] anticonvulsant,[4] antimalarial, anti-inflammatory,[5] and antidepressant.[6] The ultrasonic state increases the rate of organic changes in mild conditions that otherwise require strict pressure and temperature conditions.[7] Ultrasonic irradiation is also used to promote the formation, growth, and implosive collapse of bubbles in a liquid[8] by various synthesis reactions. Initiated by cavitation, bubble collapse causes high stresses, extreme local heating, and very short lifetimes. Cavitation acts as a way of focusing the sound's scattered energy.[9,10] Ultrasound irradiation can cause several reactions by providing activation energy, in contrast to traditional heating that provides thermal energy in the macro system.[10a] Other benefits of ultrasound irradiation include high product yields, low reaction times, minimization of side products,[10b] and nontoxic and environment-friendly solvents,[11] saving money and energy.

Previously variable methods involved synthesis of many pyrazole-4-carbonitrile derivatives via the one-pot multicomponent reaction (MCR) among arylaldehydes, malononitrile, and phenylhydrazine using appropriate catalysts.[12] The significance of such compounds and relevance of such timely topics in organic synthesis were the use of ionic liquids[13] and the need for green reaction approaches.[14] The benefit of pyrazoles in drug designing has continuously trapped the pursuit for novel and advanced methods.[15] Therefore, a novel protocol with a good and inexpensive catalyst demanding short reaction times is well desired.[16,17]

In any of the abovementioned previous studies, pyrazole-4-carbonitrile derivatives catalyzed by new Pd(II) complexes under mild conditions have not been reported. Coinciding with outlined strategies and continuation of our work, we intended to achieve another success in the catalytic history of Pd(II) complexes by synthesizing bioactive heterocyclic compounds via multicomponent reactions. Because of the the merits of being environmentally benign, readily accessible, and cost-effective,

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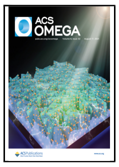

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RESEARCH ARTICLE

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Efficient and recoverable novel pyranothiazol Pd (II), Cu (II) and Fe(III) catalysts in simple synthesis of polyfunctionalized pyrroles: Under mild conditions using ultrasonic irradiation

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Abstract

Three novel Pd (II), Cu (II), and Fe (III) complexes were prepared from thiazole ligand through bidentate chelating mode. Alternative spectral and analytical tools were applied to elucidate their structural and molecular formulae. This study was extended to investigate stability and stoichiometry of complexes in solution, using standard methods. In addition, the best atomic distribution within structural forms was obtained by Material Studio Package via the density functional theory (DFT) method. This computational study fed us with significant physical characteristics for differentiation. Also, crystal surface properties in the packing system were studied using the Crystal explorer program, to evaluate the extent of contact between surfaces. Computational data discriminate Pd (II)-thiazole (HYHPd) complex by some physical features, which may be promising in the catalytic field. This complex was selected to play a catalytic function to synthesize polyfunctionalized pyrrole derivatives using ultrasonic irradiation in a one-pot reaction. The catalyst was selected for this application based on the history of Pd (II) complexes and the properties expected theoretically. A condensation reaction for aromatic aldehyde, aromatic amine, acetylacetone, and nitromethane was carried out under mild reaction conditions by ultrasonic irradiation. All reaction conditions were optimized among that variable Lewis acid catalysts in comparison to our new complexes. HYHPd catalyst displayed superiority in overall trials with high yield, short time, and green conditions (solvent H_2O/EtOH). Also, the recovery of hetero-catalyst was succeeded and reused by the same efficiency up to five times after that the efficiency was reduced. The mechanism of action was proposed based on the ability of Pd (II) for adding extra-bonds over *z* axis and supported by theoretical aspects.

KEYWORDS
benign protocol, DFT studies, HYHPd complex as recoverable catalyst, polyfunctionalizedpyrroles, ultrasonic irradiation

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Synthesis and characterization of Fe(III), Pd(II) and Cu(II)-thiazole complexes; DFT, pharmacophore modeling, *in-vitro* assay and DNA binding studies

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A B S T R A C T

New pharmacologically active complexes were prepared from Pd (II), Fe (III), and Cu (II)ions with 2-amino-6-oxo-3-(piperidinylamidino)-4-(4methoxyphenyl)-6,7-dihydro-pyrano[2,3-d]-5,7thiazol ligand (MPTP). The ligand acted as neutral bidentate with the metals *via* NH and NH_2 groups. FT-IR spectra, CHN-analysis, TGA, UV–Vis, molar conductance and ^1H &^{13}C NMR spectra were used to characterize the new compounds. Also stability constant of MPTP-complexes was identified in solution and pH-profile indicates high stability of complexes. Computational study was implemented to extract significant features for MPTP and its complexes. In addition to, essential maps were demonstrated over formulated chk-file. *In-silico* assay was executed by two different approaches over compounds to evaluate their biological behavior and degree of interaction with biological systems, before practical application. MPTPPd complex displayed priority in interaction with amino acid residues and drug-like feature. *In-vitro* assay was then carried out for compounds against different microbes and MPTPPd and MPTPCu showed high antimicrobial activity. Also, their cytotoxic behavior was examined against MCF-7, HCT-116, and HepG2 carcinoma cell lines, high cytotoxicity was clearly recorded with MPTPPd and MPTPCu complexes. Furthermore, antioxidant activity was examined and the complexes exhibited high reactivity with trapping free radicals. The interaction of metal chelates with DNA was detected by gel electrophoreses, viscosity and spectral studies. Spectrophotometric titration and viscosity studies expose that each of tested complex is an avid binder to DNA. This may be due to enhanced hydrophobic & electrostatic interaction of aromatic rings. Finally, such complexes may be considered as a promising bioactive agents.

1. Introduction

Thiazole and pyran nucleus were presented wide band of pharmacological and biologically active natural products. These are often used in biological basic building block. Most up data for thiazole fused systems, exhibit common requirements in various fields among those medicinal chemistry, as anticancer, antifungal, antibacterial and antioxidant. That in turn stimulated us to synthesize many new thiazole, pyran, and piperdine derivatives [1,2]. Thiazole ligands are designed to interact with proper metal ion to induce active metalloprotein sites [3]. Over last years, metal - drug adducts exhibiting promising therapeutic efficacy, have been focused for many investigations and are of great importance in chemistry and biology sciences. Biomolecules that having electron deficient sites (metals) can simply interact with protein or DNA according to their small sizes and high nuclear charges [4]. So many studies were carried out based on binding characteristics of d-metal complexes inside infected cells *via* either metals or ligands [5–7]. So, pharmacological efficacy of metal chelate depends primarily on metal ions and ligands coordinated [8–10]. Anticancer agents were prepared from Cu(II) complexes, due to their selective permeability for cancer cell membranes [11,12]. While, Fe(III) complexes displayed optoelectronic, catalytic and biological applications [13–15]. Potential biological and antitumor features of thiazole-complexes are based on transmembrane-glycoprotein, which describes family of tyrosine kinase receptors (TKRs) [16]. Consequently, such previous studies clarify

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Catalysis

Green Bio-organic and Recoverable Catalyst Taurine (2-aminoethanesulfonic acid) for Synthesis of Bio-active Compounds 3,4-Dihydropyrimidin Derivatives in Aqueous Medium.

Mahmoud Abd El Aleem Ali Ali El-Remaily* and Omar M. Elhady[a]

A highly green bio-organic catalyst known as Taurine (2-aminoethanesulfonic acid) is plentifully in the tissues of humans and animals and is an efficient and environmentally benign catalyst for the one-pot multicomponent reaction synthesis of bio-active 3,4-dihydropyrimidin-2(1H)-ones/thiones (Biginelli Reaction) in aqueous medium. The advantages of this protocol by way of the Taurine catalyst are that it is eco-friendly, commercially available, low cost, has high reusability, short reaction times, high yields and the products obtained high purities without using any organic solvents.

1. Introduction

In the field of catalysis, the main objective, in terms of green chemistry, is to develop environmentally friendly, commercially available, low cost, selective and efficient processes for catalyst separation and recycling.[1] Taurine (2-aminoethanesulfonic acid), is a β-amino acid with a sulfonic acid group instead of a carboxylic acid group, although it is structurally different when compared with other homologue amino acids.

Taurine is abundantly available at high concentrations in animal tissues. It is one of the constituent members of the bile present in the large intestine, the average quantity of which represents one-tenth of the total weight of the human body.[2] The name bullfighting refers to its first isolation from ox bile, termed *BosTaurus.*[3] Despite other homologues that do not dissociate at biological pH, Taurine comes in the form of a zwitterionic shape in water, which leads to essential biological and medicinal properties.[4] This formation in water is demonstrated by computation and NMR investigations.[5] Taurine is used in energy drinks, dietary supplements and also has several biological properties in the human body.[6] In addition, Taurine is used for the synthesis of barbituric and thiobarbituric acid derivatives,[7] as well as the Knoevenagel reaction in water.[8]

The Biginelli reaction proposed by Pietro Biginelli in 1891 was carried out in ethanol with an acid catalyst.[9] However; the procedure developed had a long reaction time, used not eassy reaction conditions and gave products with low yields. In last years, the reaction has been experimented by some catalysts such as mesoporous $NH_4H_2PO_4$/MCM-41,[10] sulphated polyborate,[11] sulphated tungstate,[12] zinc oxide nanoparticles,[13] N,O-bis(trimethylsilyl)acetamide, dicyclohexyl carbodiimide,[14] organosilane sulfonated graphene oxide,[15] $FeCl_3$ immobilized in Al-MCM 41[16] etc. have been used to improve reaction conditions and yields.

Biginelli synthesized dihydropyrimidin-2(1*H*)-(thi)one (DHPM) derivatives by condensation of three-component, different aromatic aldehyde, a β-keto ester and urea or thiourea. The reaction continuously attracts research interest because of the case of the DHPM moiety in various drug candidates, examples of which include the first cell-permeable antitumor scaffold, monastrol,[17] the modified analogue (*R*)-mon-97[18] and antihypertensive agent (*R*)-SQ 32,926.[19] The backbone of human life is DNA and RNA which consist of the pyrimidine derivatives. Of the five major nucleic acid bases, three are pyrimidine derivatives that include cytosine present in DNA and RNA, uracil in RNA and thymine in DNA. Owing to their participation as bases of DNA and RNA, they have become exceedingly important in the world of synthetic organic chemistry. These structures stimulated the invention of a wide range of synthetic methods for synthesis and chemical transformations. In addition to this, various important vitamins also comprise pyrimidine derivatives.[20] Thus, the importance of pyrimidones compounds to human life creates a synthetic method that is very interesting in relation to organic chemistry.

In recent years, we have worked constantly on the development of new tools and methodologies for bioactive compounds synthesised using green methodologies.[21–26]

In the present work, we used a green bio-organic and recoverable catalyst Taurine for the one-pot multicomponent reaction synthesis of bio-active 3,4-dihydropyrimidin-2(1*H*)-ones/thiones (Biginelli Reaction), an aqueous medium.

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Regular Article

Unveiling the exceptional synergism-induced design of Co-Mg-Al layered triple hydroxides (LTHs) for boosting catalytic activity toward the green synthesis of indol-3-yl derivatives under mild conditions

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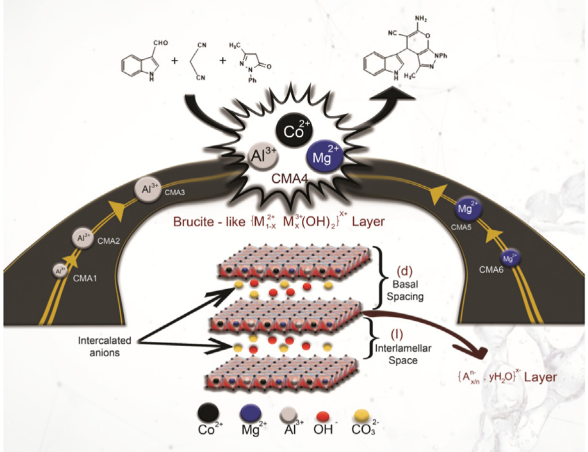
GRAPHICAL ABSTRACT



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ABSTRACT

The current study provides a novel insight into the role of synergism of the changes in Mg^{2+}/ Al^{3+} in the best catalytic activity of indol-3-yl derivatives. A series of Co-Mg-Al layered triple hydroxides (LTHs) catalysts were produced by altering the Al^{3+}/Mg^{2+} ratio with respect to Co^{2+}. The physicochemical properties of LTHs were well characterized by ICP-AES, XRD, FTIR, FE-SEM, BET, Zeta-sizer, and VSM. The results show that the sample CMA4 (Co^{2+}:Mg^{2+}:Al^{3+} 2:4:4) is an exception to the physicochemical characteristics of the produced Co-Mg-Al LTHs, which is due to the synergism between the changes in Mg^{2+} and Al^{3+}. To the best of our knowledge, this is the first study to report the synthesis of indol-3-yl derivatives from indole-3-carbaldehyde using Co-Mg-Al LTHs as highly efficient heterogeneous catalysts, which is an extremely appealing path. The selectivity of the synthesis was studied by condensing various

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RESEARCH ARTICLE

Applied Organometallic Chemistry WILEY

Rapidly, highly yielded and green synthesis of dihydrotetrazolo[1,5-*a*]pyrimidine derivatives in aqueous media using recoverable Pd (II) thiazole catalyst accelerated by ultrasonic: Computational studies

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Here, we synthesized new thiazole complexes from Cu (II), Fe (III), and Pd (II) ions. Such complexes were characterized to present their chemical formulae, firstly. The octahedral geometry was suggested for the investigated complexes except Pd (II) complex (ARPTPd), which has a square-planer arrangement. ARPTPd was planned to be used as a catalyst for synthesis of dihydrotetrazolo[1,5-*a*]pyrimidine derivatives at mild conditions. The catalytic activity of ARPTPd complex in four-components reaction approach was deliberately monitored till it reaches the most favorable conditions. The advantages of suggested catalyst were basically summarized by using green solvent (H_2O), lower reaction time, and high products yields. Also, the superiority of ARPTPd complex and ultrasonic irradiation towards synthesis of dihydrotetrazolo[1,5-*a*]pyrimidine derivatives was revealed compared with other Lewis acids, basic, and ionic liquid catalysts. Furthermore, the mildness of conversion and compatibility with different functional groups makes it attractive. In addition, in consecration, computational aspects were often taken according to their effect on the declaration or discrimination of variable functional characteristics. Crystal packing systems of complexes were configured to extract important surface properties. DFT study was also applied to explain the causes behind the superiorly of ARPTPd complex. Also, the optimization process for intermediates was executed to support the suggested mechanism. Finally, this simple, economical, and green catalytic procedure may be applied to the industry in future.

KEYWORDS
DFT, recoverable catalyst, tetrazolopyrimidine derivatives, thiazole complexes, ultrasonic irradiation

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FULL PAPER

Applied Organometallic Chemistry WILEY

Boosting the catalytic performance of zinc linked amino acid complex as an eco-friendly for synthesis of novel pyrimidines in aqueous medium

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Zinc linked amino acid complex, Zn(L-proline)$_2$, is considered as a green catalyst for the synthesis of novel series of pyrimidine derivatives **5a–q.** The pyrimidines **5a–q** were prepared via two pathways: the first is a one-pot reaction of guanidines $\mathbf{3_{a-c}}$ with aromatic aldehyde **1** and acetophenones **2**; and the second one is the reaction of guanidines $\mathbf{3_{a-c}}$ with different chalcones $\mathbf{4_{a-j}}$ in aqueous medium. The simplicity of the operation, the short reaction time, and the high efficiency (97%) are the main advantages of this protocol. Furthermore, the green aspects of this synthetic protocol were further investigated by examining the reusability of Zn(L-proline)$_2$ complex throughout five consecutive cycles without a significant loss of catalytic activity. This new procedure has presented remarkable advantages in terms of safety, simplicity, stability, mild conditions, a short reaction time, excellent yields, and high purities without using any organic solvents.

KEYWORDS
aqueous medium, benign protocol, pyrimidine derivatives, zinc linked amino acid complex, Zn (L-proline)$_2$

1 | INTRODUCTION

L-proline has been used extensively as a catalyst for enantioselective reactions such as aldol condensation.[1] The catalytic role of proline was related to the formation of an enamine with the nucleophile, which resembles the class I aldolases.[2] The complexes of various amino acids with Zn(II) have been reported by Darbre[3–5] and were also successfully used to catalyze the aldol condensation in water with a high degree of enantioselectivity. The location of the secondary amine and the carboxylate functional groups makes the proline the most prominent amino acid for coordination with Zn as soft Lewis acid. Recently, Zn(L-proline)$_2$ complex (Figure 1) emerged as a powerful catalyst for various transformations, such as aldol and nitro aldol condensation, Hantzsch condensation, and some other reactions including heterocyclic synthesis.[4,6] The Zn(L-proline)$_2$ complex can be easily synthesized via the reaction of zinc acetate Zn(AcO)$_2$ and the amino acid by using triethylamine (Et$_3$N) as a basic catalyst in methanol (MeOH) as a solvent.[3,4] The water solubility of Zn(L-proline)$_2$ and other amino acid complexes plays an important role in its function as a homogenous catalyst in mixed organic solvents and water, as it ensures sufficient solubility for both reagents involved in the reaction, while functioning simultaneously as a catalyst.

It has been shown that at least 5% water content is necessary to dissolve the Zn(L-proline)$_2$ complex.[5] This complex is almost insoluble in any other solvent, which makes the recovery of the catalyst very simple and reusable for numerous times without any activity loss.