

PROPERTIES OF PANCHARATNAM PHASE AND ENTANGLEMENT OF A FIVE-LEVEL ATOM INTERACTING WITH A SQUEEZED FIELD

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Abstract

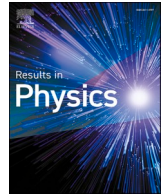
We introduce a quantum scheme where a single five-level atom interacts with a single-mode cavity field by a time-dependent coupling. During the interaction, the temporal behavior of the quantum entropy in the atomic basis is compared with that of the Mandel parameter used to quantify the nonclassical properties of the field. With the field prepared in a squeezed coherent state, the atomic quantum entropy is then used to quantify the entanglement or the nonlocal correlation of the five-level atom (5LA)–field system. The influence of one- and two-photon transitions and the atomic motion on the degree of entanglement and the Pancharatnam phase is analyzed. The analysis emphasizes that both the time dependence and photon multiplicity play an important role in the evolution of the degree of entanglement, the Pancharatnam phase, and nonclassical properties. This insight may be very useful in various applications in quantum physics and quantum optics.

Keywords: five-level atom, linear entropy, atomic motion, squeezing parameter, photon multiplicity.

1. Introduction

Essential features in quantum mechanics, namely, the Pancharatnam phase (PP) and the geometric phase (GP) have been studied by many physicists [1–5]. Michael Berry demonstrated that the quantum object – the wave function (WF) – maintains its evolution in the complex-valued argument of the WF, namely, the GP factor. In regard to its dynamical influence, the GP factor depends on the path geometry of the scheme that the quantum object traverses [6]. This factor is stable despite the uncertainties in control and environmental perturbations. Therefore, researchers pay it close attention while conducting fault-tolerant quantum computations. Focusing on the generalized Heisenberg algebra coherent state (CS), we have recently explored the PP and the purity of the field for several quantum systems [7, 8].

In this context, the link between the GP and field purity is highly sensitive to the photon transition number and the initial atomic state. In regard to the atomic motion, the influence of a time-dependent



Properties of transient spectrum and field purity for a qubit system in squeezed states

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ARTICLE INFO

Keywords:

Squeezed coherent states
Squeezed number states
Transient spectrum
Field purity

ABSTRACT

The present study investigates the transient spectrum (TS) of a two-level system that interacts with a generalized squeezed state without using the rotating wave approximation (RWA). We consider the purity of the optical field, which is developed in a generalized squeezed state, utilizing the linear entropy. The analytic expressions of the TS and field purity (FP) of the bipartite system are evaluated. Moreover, the study exhibits the influence of the squeezed parameter and some photons transition on the TS and FP. We obtain that the control of the FP may be generated based on an adequate choice of the photons transition and squeezed parameter. Such results can be utilized in the understanding and development of various tasks of quantum physics and optics.

Introduction

The abrupt radiation is considered as a primary reason of energy relaxation in an environmentally-coupled quantum system. However, it can be controlled by changing the field affects the quantum system [1], referred to as the Purcell effect. Enclosing the qubits in a cavity resonator that is detuned from the qubit frequency has resulted in improving the qubit lifetime while keeping qubit control [2–4]. Such dispersive coupling amid the qubit and the resonator plays a role in reducing the channels of decay close to the qubit frequency. However, these channels should undergo additional suppression. Contemporary authors have benefited from these techniques in the mismatches of engineering impedance in the Purcell decay channels existing in the resonator [5,6].

The photon, as a concept, in the quantum theory pertaining to a radiation field relied on the number (Fock) state. Nonetheless, the coherent states are also significant, which are defined as a linear superposition of the Fock states with choosing coefficients. In this case, the states can be generated by acting the displacement operator on the vacuum state [7–9]. Recently, squeezed states have played an important role in the development of various tasks of quantum technology. These states are classified as non-classical states in quantum optics that can be generated by using the operation of the squeezed operator [10]. Squeezed displaced Fock states were developed and their various features, including squeezing and photon statistics were explored [11,12]. They extend two-photon coherent states [13] (squeezed coherent states), squeezed number states [14] and displaced Fock states [15].

Lately, authors have reported the development of motion of a trapped ion in nonclassical states, e.g. Fock states, coherent states, squeezed states and Schrödinger-cat states [16,17].

The JCM (Jaynes Cummings model) has fulfilled the foundation of the nonclassical states through the conditional measurement method [16]. Dakna, Knoll and Welsch (1998) have provided a review for further details relevant to JCM [17]. The development of coherent states with JCM is a significant issue because it provides the information about the non-classical effects that depend on the kinds of the interaction between atoms and fields, including the cases of Schrödinger-cat states [18], displaced number states [19] and squeezed coherent states [20]. It has been shown that the squeezed parameter significantly affects the dynamical properties of the field primarily in the squeezed coherent state [21]. Recent works have shown the effect of the squeezed parameter on the entanglement for a system of two 3LAs (three-level atoms) interacting with a squeezed field [22]. The dynamical properties of a 3LA coupled to a field mode primarily developed in the squeezed coherent state without using the RWA have investigated [23,24]. The effect of the atomic motion within center-of-mass wave functions and atom nanolithography has examined [25]. Recently, the emission spectrum of an optical radiation field interacting with a 2LA when this field is initially in the coherent states (CSs) of added photons associated with pseudo-harmonic oscillators has discussed [26]. Moreover, it has found that the emission spectrum is extremely sensitive to the deformed field and detuning parameters [27]. More recently, a link between the emission spectrum and quantum state fidelity for an atomic system

<https://doi.org/10.1016/j.rinp.2021.104297>

Received 22 October 2020; Received in revised form 2 May 2021; Accepted 4 May 2021

Available online 11 May 2021

2211-3797/© 2021 The Authors.

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Radial vibrations on an elastic medium subjected to rotation and magnetic field

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ABSTRACT

Based on the one-dimensional elastic theory, the radial vibrations of cylindrical isotropic embedded in an elastic medium are studied in the paper. The effect of the magnetic field of the radial vibrations of an elastic hollow cylinder with rotation is researched as well. The one-dimensional equation of elastodynamic is solved in terms of radial displacement. The frequency equation is obtained when the boundaries are free and fixed; the mixed boundary condition is numerically examined. The determination is concerned with the eigenvalues of the natural frequency of the radial vibrations in the case of harmonic vibrations. The effect of the magnetic field and rotation on the natural frequencies were explored. It was shown that the dispersion curves of guided waves were significantly influenced by the magnetic field and rotation of the elastic cylinder. Numerical results are given and graphically illustrated in each considered case. The natural frequencies and mode shapes are calculated numerically, and the effects of rotating, magnetic field, and variable thickness are discussed. It is observed that an increase of the magnetic parameter, as well as the rotation parameters, brings results closer to the classical cylinder theory results. Furthermore, the current study can be applied to the design of microplates and nanoplates and their optimal usage. The results indicate that the effects of the magnetic field and rotation are very pronounced.

ARTICLE HISTORY




Received 16 December 2020
Accepted 10 January 2021

KEYWORDS

Elastodynamics; radial vibrations; isotropic material; magnetic field; rotation; elastic; hollow cylinder

1. Introduction




In the past, accidental failure of rotating cylinder wheels due to flexural vibration has frequently occurred in rotodynamic machinery such as steam turbines and gas turbines. Wang, Wang, and Liu (2020) investigated the mechanical magnetic coupling vibration instability of an angular rotor subjected to synchronous load in axial-flux permanent magnet motors. Lu, Tsouvalas, and Metrikine (2019) studied the vibration of higher-order model for in plane vibrations of rotating rings on an elastic foundation. Shojaeefard et al. (2018) studied the free vibration problem of an ultra-fast-rotating-induced cylindrical nanoshell resting on a Winkler foundation under a thermo-electro-magneto-elastic condition and recommended some protective measures. Sobhy and Zenkour (2018) investigated the effect of the magnetic field on the thermomechanical buckling and vibration of viscoelastic sandwich nanobeams in humid environment. Zhu et al. (2020) discussed the axisymmetric torsional and longitudinal vibrations for an incompressible SEA cylindrical tube under inhomogeneous biasing fields induced by radial electric voltage and axial pre-

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Communicated by Dr Krzysztof Kamil Zur.

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Article

Regression Models to Estimate Accumulation Capability of Six Metals by Two Macrophytes, *Typha domingensis* and *Typha elephantina*, Grown in an Arid Climate in the Mountainous Region of Taif, Saudi Arabia

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Citation: Al-Sodany, Y.M.; Saleh, M.A.; Arshad, M.; Abdel Khalik, K.N.; Al-Bakre, D.A.; Eid, E.M. Regression Models to Estimate Accumulation Capability of Six Metals by Two Macrophytes, *Typha domingensis* and *Typha elephantina*, Grown in an Arid Climate in the Mountainous Region of Taif, Saudi Arabia. *Sustainability* **2022**, *14*, 1. <https://doi.org/10.3390/su14010001>

Received: 4 December 2021

Accepted: 13 December 2021

Published: 21 December 2021

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Abstract: In this study, we explored the capacity for two promising macrophytes, *Typha domingensis* and *Typha elephantina*, to be used for the surveillance of contamination by six metals, i.e., Cu, Fe, Mn, Ni, Pb, and Zn, in the mountainous area of Taif City in Saudi Arabia. Regression models were generated in order to forecast the metal concentrations within the plants' organs, i.e., the leaves, flowers, peduncles, rhizomes, and roots. The sediment mean values for pH and the six metals varied amongst the sampling locations for the respective macrophytes, indicating that similar life forms fail to indicate equivalent concentrations. For instance, dissimilar concentrations of the metals under investigation were observed within the organs of the two rooted macrophytes. The research demonstrated that the segregation of metals is a regular event in all the investigated species in which the metal concentrations vary amongst the different plant constituent types. In the current study, *T. domingensis* and *T. elephantina* varied in their capacity to absorb specific metals; the bioaccumulation of metals was greater within *T. domingensis*. The relationships between the observed and model-estimated metal levels, in combination with high R^2 and modest mean averaged errors, offered an appraisal of the goodness of fit of most of the generated models. The *t*-tests revealed no variations between the observed and model-estimated concentrations of the six metals under investigation within the organs of the two macrophytes, which emphasised the precision of the models. These models offer the ability to perform hazard appraisals within ecosystems and to determine the reference criteria for sediment metal concentration. Lastly, *T. domingensis* and *T. elephantina* exhibit the potential for bioaccumulation for the alleviation of contamination from metals.

Keywords: bioaccumulation and translocation factors; bioaccumulators; cattails; environmental pollution; macrophytes; prediction models; wetlands

1. Introduction

Metals are a specific class of elements that, in contrast to organic contaminants, are unable to be broken down via biological processes [1]. Owing to their adverse impact

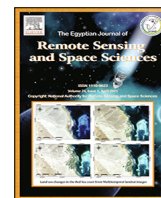
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The Egyptian Journal of Remote Sensing and Space Sciences

journal homepage: www.sciencedirect.com

Remote sensing-based geological mapping and petrogenesis of Wadi Khuda Precambrian rocks, South Eastern Desert of Egypt with emphasis on leucogranite

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ARTICLE INFO

Article history:

Received 7 March 2019

Revised 10 July 2019

Accepted 11 July 2019

Available online 19 July 2019

Keywords:

Leucogranites

Khuda

I-type

Remote sensing

Eastern Desert

Egypt

ABSTRACT

The exposed Precambrian rocks along Wadi Khuda area, South Eastern Desert of Egypt, comprise gneisses, amphibolites and migmatites associations (infrastructural rocks) which are intruded by diorite, tonalite, syenogranite and leucogranite (LG). LG forms homogeneous boss like bodies, devoid to xenoliths, except along the outer margins. Chemically and mineralogically they are dissimilar to the surrounding gneisses. In the current study, band ratio and Decorrelation Stretch image processing algorithms were proposed and applied on Landsat-8, Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) and Sentinel-2 remote sensing data to discriminate the widely exposed lithological units in the mapped area. Geochemically, I-type classification and volcanic arc environment were revealed. LG is peraluminous (ASI average of 1.09) with normative corundum up to 1.38 for LG. The LG displays limited major and trace element variations ($\text{SiO}_2 = 74.5\text{--}76.2\%$, $\text{Al}_2\text{O}_3 = 13.4\text{--}14.4\%$, $\text{MgO} = 0.03\text{--}0.19\%$, $\text{Na}_2\text{O} = 3.6\text{--}4.6\%$, and $\text{Rb} = 55\text{--}85$ ppm) probably due to textural and mineralogical homogeneity. The contents of REE in the leucogranite are low ($\sum\text{REE} = 21\text{--}37$), but the REE patterns are $[(\text{La}/\text{Yb})_n = 2.45\text{--}9.03]$, $[(\text{La}/\text{Sm})_n = 1.09\text{--}2.6]$, with negative Eu anomaly, $(\text{Eu}/\text{Eu}^* = 0.19\text{--}0.78)$. The negative Eu anomaly and the low Sr content (16–92 ppm) may be attributed to the plagioclase feldspars fractionation. The leucogranites represent residual melt of syenogranite which forms Um Itly pluton at the southern flank of Wadi Khuda entrance.

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1. Introduction

The Egyptian granites are differentiated into grey and pink types (e.g. El-Gaby et al., 1988, 1990). The grey (older) granite type was emplaced during the Pan-African Orogeny (i.e. Syn-orogenic) and are of I-type granites (Chappell and White, 1974). The monzogranites and syenogranites were emplaced during post Pan-African event which are referred to the younger (pink) granite type (Late to post orogenic) which is mostly equivalent to A-type granite (Chappell and White, 1974). The S-type granite was proposed to some granites at the Eastern Desert of Egypt e.g. Sikait area (Mohamed and Hassanen, 1997) and the El-Hudi area (Moghazi et al., 2001), where they are distinguished by their chemical and

mineralogical characters (Fig. 1). There are several hypotheses concerning the mode of formation, evolution and tectonic setting of the granitic melts, some of these mechanism considered the interaction between mantle and the lower crust (e.g. Pitcher, 1983). Therefore, the granitic rocks could be formed by anatexis and/or fractional crystallization (FC) processes of lower crust and subduction related magmatism respectively (Stern and Hedge, 1985; Stern and Abdelsalam, 1998; El-Gaby et al., 1990; Fritz et al., 2002; Johnson and Woldehaimanot, 2003; Heikal et al., 2019). Granitic rocks with crustal components have been differentiated from the mantle-derived types in arc-type and/or at an active continental margin (Abdel-Rahman and Martin, 1990).

Remote sensing data such as ASTER, Sentinel-2 and Landsat-8 were used for lithological mapping in the Eastern Desert of Egypt (e.g. Gabr, et al., 2015; Hassan and Ramadan, 2015; Hassan, et al., 2015; Hassan and Sadek, 2017; Hassan et al., 2017; Ali-Bik, et al., 2018).

Peer review under responsibility of National Authority for Remote Sensing and Space Sciences.

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<https://doi.org/10.1016/j.ejrs.2019.07.004>

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Reservoir Formation Damage; Reasons and Mitigation: A Case Study of the Cambrian–Ordovician Nubian ‘C’ Sandstone Gas and Oil Reservoir from the Gulf of Suez Rift Basin

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Received: 13 September 2020 / Accepted: 14 July 2021
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Abstract

Reservoir formation damage is a major problem that the oil and gas industry has to mitigate in order to maintain the oil and gas supply. A case study is presented that identifies the impacts of formation damage and their causes in the Nubian ‘C’ hydrocarbon reservoir within Sidki field located in the Southern Gulf of Suez, Egypt. In addition, a formation damage mitigation program was designed and implemented involving an effective stimulation treatment for each well experiencing reservoir damage. The data available for this study include core analysis to provide rock mineralogy and lithology; analysis of production fluid data; water chemistry; drilling fluid composition; perforations and well completion details; workover operations; and stimulation history. The diagnosis of formation damage based on the integrated assessment of the available data is associated with several benefits, (1) The integration of the data available helps provide a robust analysis of formation damage causes and in establishing suitable remediation actions, (2) Workover fluid is confirmed as the primary cause of reservoir damage in the studied well, (3) Several reservoir damage mechanisms were identified including water blockage, solids and filtrate invasion, fluid/rock interaction (deflocculation of kaolinite clay), salinity shock and/or high-sulfate content of the invaded fluid, (4) Irrespective of the potential causes of formation damage, the primary objective of a gas production company is to mitigate its effects and the integrated dataset helps to design appropriate and effective stimulation treatments to overcome formation damage, and (5) In gas reservoirs, especially low permeability ones, extra precautions are necessary to avoid potential reservoir damage due to workover fluid invasion.

Keywords Reservoir damage analysis · Formation damage · Reservoir damage reasons · Reservoir damage mitigation · Nubia sandstone reservoir · Gas reservoir · Workover Formation damage · Fines migration · Well stimulation · Fluid invasion · Water blockage · Overbalanced workover · Integrated formation damage assessment workflow

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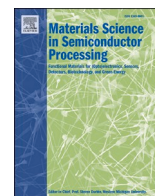
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1 Introduction

Formation or reservoir damage is a challenging issue in oil and gas industry that can substantially reduce fluid flow rates and recovery from subsurface reservoirs [1–6]. It typically involves the reduction in the near-wellbore permeability leading to a reduction in the well productivity. It is a relatively frequent outcome of operations conducted on wellbores during drilling, workover, production, stimulation programs and/or other actions designed to enhance gas or oil recovery (EOR) [3–10]. Many authors have investigated the potential causes of formation damage, and a number of distinct potential causes have been identified in relation to the various downhole activities carried out in gas and oil boreholes [ex 3, 4, 6, 11–30]. Reservoir damage involves





Role of Cu dilute on microstructures, optical, photoluminescence, magnetic and electrical properties of CdS film

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ARTICLE INFO

Keywords:

Thin films
CdS_{1-x}Cu_x films
Microstructural parameters
Optical parameters
PL spectra
Hysteresis loop
Electrical properties

ABSTRACT

Thin films of CdS_{1-x}Cu_x (with $0 \leq x \leq 0.10$) were deposited using electron beam evaporation. Using XRD, EDX, SEM and UV-Vis-NIR spectroscopy, the impact of [Cu]/[S] on the film properties was examined. The influences of various concentrations of Cu are also elucidated on the optical parameters of the films. The XRD analysis shows that the thin films of CdS_{1-x}Cu_x have been improved and have hexagonal polycrystalline structure with the increase of Cu doping ratio. Additionally, the crystallite size is reduced while the micro-strain ϵ increases with enhancement of the incorporation of Cu in CdS lattice. The envelope method was used to extract the optical parameters of the undoped and Cu-doped CdS films. With the increase of Cu concentration, the energy optical bandgap decreased, and the variation values of band gap could play an important role in solar cell applications. Another optical parameters such as, dissipation factor and real/imaginary dielectric constant parts were evaluated and demonstrated a strong Cu doping dependence. The shift observed in the photoluminescence spectra emission band confirmed Cu's substitution to CdS lattice. The measurements of magnetization using vibrating sample magnetometer illustrated a hysteresis loop in Cu-doped CdS films, and confirmed the room temperature ferromagnetism. Finally, the Hall effect results show that the pure CdS film corresponds to an n-type semiconductor with a resistivity of $8.11 \times 10^{-2} \Omega \text{ cm}$ and a carrier concentration of $29.6 \times 10^{19} \text{ cm}^{-3}$, and the CdS:Cu film is a p-type semiconductor and the resistivity is reduced from 6.8×10^{-2} to $3.7 \times 10^{-2} \Omega \text{ cm}$, and the carrier concentration is reduced from 26.4×10^{19} to $4.1 \times 10^{19} \text{ cm}^{-3}$, which has potential application prospects in solar cells.

1. Introduction

Semiconductor group II – VI doped with transition metals as cobalt (Co), vanadium (V) manganese (Mn), copper (Cu), etc, are essential for their fundamental role of in solar cells manufacture and advanced research materials and technological applications [1,2]. Among these, CdS is very important semiconductor that providing energy gaps of 2.57 eV (in hexagonal phase and 2.42 eV (in cubic phase) at room temperature (RT). In addition, these semiconductors materials possess the interesting properties which qualify them to be utilized in recent different optoelectronic applications such as lasers, visible-light emitting diodes, non-linear optics and modern solar cells of high efficiency [3,4].

Doping CdS semiconducting materials with Cu impurities could lead

to large variations of the resistivity, band gap energy, photo-electrical properties and also altering the type of semiconductor from “n-type to p-type” [5,6]. In fact, the presence of copper atoms in semiconductors are affected many interesting physico-chemical properties and reduce electrical resistance as Cd-S thin films have very high electrical resistance (10^7 – $10^8 \Omega \text{ cm}$) [7,8]. On the other side, the optical properties of doped nano-materials vary from the corresponding host nano-materials as the dopants form deep trap levels serve as luminescence centers. Just a few reports have been published on Cu²⁺ doped Cd-S nanoparticles [9, 10]. As mentioned above, the semiconducting materials doped with a low amount of metal impurities have unique properties that make them important materials for potential applications, yet another purpose is to enhance the optical properties of Cd-S film doping with metal ions. The CdS and CdS:Cu thin films have been prepared by several growth

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<https://doi.org/10.1016/j.mssp.2021.105687>

Received 1 September 2020; Received in revised form 10 January 2021; Accepted 11 January 2021

Available online 17 January 2021

1369-8001/© 2021 Published by Elsevier Ltd.



Cite this: *Environ. Sci.: Processes Impacts*, 2021, 23, 1006

Sea urchin-like calcium borate microspheres and synergistic action with cholinesterase-inhibiting insecticides for ecofriendly *Spodoptera littoralis* control†

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The development of nanoagrochemicals has attracted much attention in the last decade to overcome the recent agricultural and environmental challenges associated with the intensive usage of insecticides. Herein, nanostructured calcium borate materials with hierarchical sea urchin-like microspheres and microblocks have been synthesized by a facile hydrothermal method. The insecticidal activity of CaB_2O_4 and its synergistic combination with cholinesterase-inhibiting insecticides are explored against *Spodoptera littoralis* (*S. littoralis*) for the first time via a feeding bioassay protocol. The insecticidal efficacy of sea urchin-like microspheres (CB-A) is estimated to be $\text{LC}_{50} = 207 \text{ mg L}^{-1}$ which is two-fold higher than that of microblocks (CBM-A) with $\text{LC}_{50} = 406 \text{ mg L}^{-1}$ after eleven days of exposure. The synergistic combination of the CB-A sample with methomyl and chlorpyrifos increases the toxicity to 2.4 and 2.6-fold higher than that of the individual insecticides, respectively. Significantly, sea urchin-like CaB_2O_4 microspheres cause physical damage to the external insect's cuticle layer, which consequently enhances the uptake of organic insecticides. Our results revealed that calcium borate micro-/nano-structures can be employed as a multifunctional nanoagrochemical in various agricultural programs for *S. littoralis* control and decrease the usage of cholinesterase-inhibiting insecticides.

Received 22nd March 2021
Accepted 14th May 2021

DOI: 10.1039/d1em00125f

rsc.li/espi

Environmental significance

Sea urchin-like CaB_2O_4 microspheres have been synthesized by a facile hydrothermal approach. The insecticidal activity of CaB_2O_4 and its synergistic combination with cholinesterase-inhibiting insecticides *i.e.* methomyl and chlorpyrifos against *Spodoptera littoralis* are explored for the first time. CaB_2O_4 showed high insecticidal activity not only on the larvae stage but also on pupa and adult stages. The combination of CaB_2O_4 with methomyl and chlorpyrifos increased the toxicity to 2.4 and 2.6-fold higher than that of the individual insecticides, respectively. CaB_2O_4 with a sea urchin-like morphology causes physical damage to the cuticle layer and enhances the penetration of organic insecticides and consequently the loss of water content. Our results revealed that calcium borate with a sea urchin-like morphology can be employed as a multifunctional nanoagrochemical in various agricultural programs for *S. littoralis* control and decrease the usage of cholinesterase-inhibiting insecticides.

1. Introduction

Spodoptera littoralis (Boisduval) (Lepidoptera: Noctuidae) is one of the foremost phytophagic damaging insects in Egypt and Africa due to its high generative rate. It feeds on forty plant families and at least eighty-seven different plant species. Several cultivated plants and crops such as cotton, maize, potatoes, cereals, vegetables, and ornamental plants are extensively devastated.¹ Although *S. littoralis* is native to Africa, it spreads

all over the world. Therefore, the European and Mediterranean Plant Protection Organization (EPPO) registered *S. littoralis* as an A2 quarantine pest and alerted it as a highly invasive species in the United States.² Carbamates and organic phosphorus compounds (OPs) are well-known organic insecticides widely used for *S. littoralis* control due to inhibiting the cholinesterase enzyme activity that is responsible for the proper function of an insect's nervous system.³ However, the intensive application of organic insecticides increases the public awareness of their severe risk to human health and the environment. As a result, the Environmental Protection Agency (EPA) banned several organic insecticides.^{4,5} Many researchers and agrochemical companies devoted their interest to developing efficient and sustainable strategies for insect control.⁶ Due to the nano-science revolution, engineering nanomaterials might provide

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† Electronic supplementary information (ESI) available. See DOI: 10.1039/d1em00125f

RESEARCH

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Seasonal shape variations, ontogenetic shape changes, and sexual dimorphism in a population of land isopod *Porcellionides pruinosus*: a geometric morphometric study

Tarek G. Ismail

Abstract

Background: Isopods shape features are sensitive and respond to several selective pressures which may result in variations of these features. These pressures might reflect the heterogeneity of the environment where an animal lives. Land isopods *Porcellionides pruinosus* were collected from an agricultural field. Landmarks geometric morphometrics was applied to evaluate its shape changes during two different seasons. The present work aims to (i) assess and characterize morphological changes in body shape of *P. pruinosus* as a response to seasonal variations, (ii) determine differences in the body shape during ontogeny, (iii) examine the effect of intraspecific allometry to interpret the observed variations in the species, and (iv) clarify whether the body shape of *P. pruinosus* can be used as a sexual differentiating trait.

Results: Juveniles showed no seasonal variations in the body shape, which were detected among adults, females and males as shown by PCA, DFA, and MANOVA.

The adult winter forms have large bodies, small heads, broad pereons, and short but wide telsons. The adult summer forms have small slender bodies, slightly stretched heads, and relatively long telsons. Juveniles' growth to adulthood showed body shape changes in the head and pereon, that include shrank of the head in the anteroposterior direction and its level became slightly lower than the body. The pereon becomes broader and the two anterolateral projections of the first pereonite extend anteriorly, reaching a little beyond the posterior margin of the eyes. Present species showed a shape sexual dimorphism which includes the broader body and more convex pereon in females and a small waist between the second and third pleonites in males. Shape sexual dimorphism was attributed to reproductive activity. Both allometric trajectories of juveniles and adults (ontogenetic allometry) and of sexes (static allometry) were parallel.

Conclusions: The landmark geometric morphometric technique was able to reveal the seasonal shape variations in terrestrial isopod *P. pruinosus*. Also, this method provides information about shape variations between juveniles and adults, as well as about shape sexual dimorphism.

Keywords: Isopoda, Body shape variations, Geometric morphometric, Seasonal effects, Ontogeny, Sexual dimorphism

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Secondary minerals in a calcareous environment: an example from Um Gheig Pb/Zn mine site, Eastern Desert, Egypt

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Received: 25 August 2020 / Accepted: 15 March 2021 / Published online: 25 March 2021
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Abstract

Alteration of abandoned mine sites and wastes generates variable secondary mineral phases that incorporate different toxic trace elements with a prospective threat to the neighboring ecosystems. The main focus of this study was to investigate the mineralogical and geochemical changes at neutral pH where dry condition prevails around oxidation-primary contacts interface and the surface in Um Gheig Pb/Zn mine, Eastern Desert, Egypt. The secondary minerals were determined by M4 Tornado μ -EDXRF, Raman microscope and scanning electron microscopy with energy-dispersive system. Two alteration zones were recognized depending on ion availability and the Eh/pH conditions. The first include anglesite as an initial phase that quickly transformed into a more stable cerussite and hydrocerussite. Mendipite formation was controlled by the availability of Cl^- ions in the solution. Hemimorphite was formed after sphalerite in the pore spaces, depending on the accessibility of Si ions from silicates dissolution. Iron (oxy) hydroxides were formed in a later stage due to their restricted mobility in carbonates. The second zone includes gypsum and anhydrite formed at the surface of the mine wastes due to continuous evaporation in arid environments. These secondary mineral phases can undergo different mineral transformations depending on the prevailing conditions. The element release ratios in the mine surface zone compared to the capillary fringe zone reached 12.1, 2.8, 1.6, 0.17, 0.09 and 0.03 for Sr, Cr, Pb, Zn, Cu, and Ni in the mine surface zone compared to 5.86, 0.01, 0.05, 0.02, 0.07 and 0.01 in the capillary fringe zone. The findings from this investigation have important implications for the management and the control of elements mobility from secondary phases formed in mined areas.

Keywords Mine wastes · Secondary minerals · Arid environments · Pb/Zn mine · Eastern Desert · Egypt

Introduction

Abandoned mining sites cause many environmental issues to the nearby soil and surface/groundwater resources worldwide (Younger et al. 2002; Khelifaoui et al. 2020). After mining operations cease, pyrite (FeS_2) and other metal sulfides located in the mine wastes undergo oxidation after exposure to atmospheric oxygen. The oxidation mechanism depends on many factors including the mineralogy and reactivity of sulfides and carbonates, the particle size, porosity and surface area, the climate including the temperature and water content, the Eh/pH conditions and microbiological

activity (Nordstrom and Alpers 1999; Rammlmair et al. 2008; Redwan et al. 2012; Oyewo et al. 2018). Mine wastes can generate after oxidation acidic water rich in different metals, which are potential eco-toxicants (Jambor 1994). If carbonate is present, the acidity is buffered by carbonate minerals dissolution, resulting in co-precipitation of secondary mineral phases (Blowes and Ptacek 1994; Oyewo et al. 2018) depending on the chemical constitution of the primary wastes and the prevailed conditions. The secondary minerals act as sinks for toxic trace elements and remove them by precipitation (e.g., as hydroxides), coprecipitation, or surface-reactive iron (oxy) hydroxides or sorption onto organic material (Dzombak and Morel 1990; España et al. 2005; Alakangas and Öhlander 2006; Schaidler et al. 2014).

Natural attenuation mechanisms by absorption and precipitation of toxic trace elements or valuable economic trace elements that can accumulate as amorphous or micro-to crystalline phases within tailings and waste materials (Graupner et al. 2007; Rammlmair et al. 2008; Redwan et al.

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**PHYSICS OF NUCLEI
AND ELEMENTARY PARTICLES**

Sensitivity of Polarization Observables in $\gamma d \rightarrow \pi^0 d$ Reaction Near Threshold to the Choice of Elementary $\gamma N \rightarrow \pi N$ Amplitude and Deuteron Wave Function

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Received January 03, 2021; revised February 28, 2021; accepted March 11, 2021

Abstract—We study the sensitivity of polarization observables in $\gamma d \rightarrow \pi^0 d$ reaction near threshold to the choice of elementary $\gamma N \rightarrow \pi N$ amplitude and NN potential model adapted for the deuteron wave function (DWF). Numerical results for various beam, target, and beam–target polarization observables are presented and systematic uncertainties caused by the use of different elementary operators and DWFs are evaluated. The calculations are based on a $\gamma d \rightarrow \pi^0 d$ approach in which realistic models for the elementary pion production amplitude and the DWF are used. We find considerable dependencies of the estimated results for all possible polarization observables on the elementary amplitude. The spin asymmetries Σ , T_{21}^c , T_{10}^l , and T_{20}^l show large sensitivities to the DWF. In contrast, the asymmetries T_{11} , T_{2M} ($M = 0, 1, 2$), T_{10}^c , and E as well as the helicity difference $d(\sigma^P - \sigma^A)/d\Omega$ have slight dependence on the DWF only at photon energies very close to π -threshold. The unpolarized differential cross section is also predicted and compared with the available experimental data, and a satisfactory agreement is obtained only at forward pion angles. We expect that the results presented here may be useful to interpret the recent measurements from Jefferson Lab, TAPS@ELSA, A2 and GDH@MAMI Collaborations.

Keywords: meson production, photoproduction reactions, few-body systems, deuteron, polarization phenomena in reactions, spin observables, polarized beams, polarized targets.

DOI: 10.3103/S0027134921030036

1. INTRODUCTION

Meson electromagnetic production on light nuclei is of fundamental interest and thus constitute a major topic in medium energy nuclear physics with respect to the following important reasons: (i) used to investigate the structure of hadrons in the nonperturbative domain of quantum chromodynamics (QCD) and therefore the nature of strong interactions, (ii) study of the behavior of nucleon resonances in the nuclear medium, (iii) yields important information about πN and NN interactions as well as the electromagnetic properties of elementary particles, (iv) gives complementary information on pion production on off-shell nucleons which is important for the study of pion production on all other nuclei as well, (v) provides us with a wealth of important information about the role of the nuclear environment on the elementary amplitudes,

and (vi) serves as a test of our understanding of the chiral πN dynamics.

Coherent pion photoproduction on the deuteron is worth to be studied, since relevant experimental studies are performed [1–30]. This process may be used as an isospin filter and it is sensitive to the coherent sum of the proton and neutron amplitudes $\gamma p \rightarrow \pi^0 p$ and $\gamma n \rightarrow \pi^0 n$, respectively. The use of deuteron as an effective neutron target allows one to obtain abundant information about the mechanisms of the elementary pion photoproduction on the free neutron which otherwise is not possible due to the absence of any free neutron targets. Furthermore, the deuteron represents also an ideal object for the study of NN interactions.

During the last decades, coherent π^0 -photoproduction on the deuteron has been studied extensively in the photon lab-energy region from π -threshold up to 1 GeV as a source of information on π^0 -photoproduction off the neutron [31–62]. Despite all

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Simultaneous biodegradation of harmful *Cylindrospermopsis raciborskii* and cylindrospermopsin toxin in batch culture by single *Bacillus* strain

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Received: 25 January 2021 / Accepted: 16 August 2021 / Published online: 21 August 2021
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Abstract

This study investigates the capability of a *Bacillus flexus* strain isolated from decayed cyanobacterial blooms for the bioremediation of *Cylindrospermopsis raciborskii* and cylindrospermopsin (CYN) toxin. The algicidal activity of this strain was tested by co-cultivation with *C. raciborskii* cultures. CYN biodegradation was investigated in the presence of living and heat-inactivated bacterial cells or bacterial filtrate. Living bacterial cells inhibited *C. raciborskii* growth after 2 days of incubation with complete cell death at day 5. Bacterial filtrate caused a rapid reduction in *C. raciborskii* growth at the first day, with complete cell lysis at day 3. Only living cells of SSZ01 caused reduction in CYN released into the medium during the bacterial decay of *C. raciborskii* cells. The biodegradation rate of CYN by SSZ01 relied on initial toxin concentrations. The highest rate ($42 \mu\text{g CYN L}^{-1} \text{ day}^{-1}$) was obtained at the higher initial concentration ($300 \mu\text{g L}^{-1}$), and the lowest ($4 \mu\text{g CYN L}^{-1} \text{ day}^{-1}$) was at lower concentration ($50 \mu\text{g L}^{-1}$). These results suggest that this bacterial strain could be employed to bioremediate cyanobacterial blooms in freshwaters. Also, the application of this bacterium in slow sand filters would give possibilities for degradation and bioremediation of cyanotoxins in drinking water treatment plants.

Keywords Bacteria · Biodegradation · Biological control · *Cylindrospermopsis* · Cylindrospermopsin · Lysis

Highlights

- We proved the lytic activity of *Bacillus flexus* SSZ01 against *C. raciborskii*
- The lytic activity was mediated by bacterial secretion of active metabolites
- Strain SSZ01 can also degrade CYN toxin released from decayed cyanobacterial cells
- This strain could be used as a bioagent to control *C. raciborskii* bloom in water
- The strain could be applied in slow sand filters to remove CYN from drinking water

Responsible Editor: Vitor Vasconcelos

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Introduction

Harmful cyanobacterial blooms (HCBs) seriously threaten the environmental and human health. HCBs are a common phenomenon in freshwater environments worldwide, and they may increase in the future because of progressive eutrophication of aquatic ecosystems and climate change (Paerl and Otten 2013). Most cyanobacterial blooms are constituted by toxin-producing species which damage the aquatic ecosystem and impair the safety of drinking water (Mohamed and Al-Shehri 2007; Mohamed et al. 2015). Among bloom-forming cyanobacteria, *C. raciborskii* is one of the most common and widespread species, and characterized by geographic expansion due to its high plasticity and physiological tolerance to a wide range of environmental conditions, e.g., light, temperature, and nutrients (Padisak 1997; Burford and Davis 2011). Additionally, *C. raciborskii* can produce hepatoxins (e.g., cylindrospermopsin) and neurotoxins (saxitoxins) that have been implicated in fish, domestic livestock, and human mortalities (Svircev et al. 2016).

CYN is an alkaloid toxin with a low molecular weight (415Da), inhibiting protein synthesis (Van Apeldoorn et al.



Structural, optical and electrical properties of $\text{Bi}_{2-x}\text{Mn}_x\text{Te}_3$ thin films

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Received: 17 July 2021

Accepted: 21 October 2021

Published online:
1 November 2021

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ABSTRACT

Undoped and Mn doped Bi_2Te_3 ($x = 0, 0.05$ and 0.10 at%) thin films were prepared via thermal evaporation method from their bulk alloys. X-ray diffraction revealed the presence of hexagonal Bi_2Te_3 crystalline phase only in all undoped and Mn doped films. EDAX quantitative analysis revealed that the effective Mn doping is close to that of the intended. SEM observations revealed uniform spherical grains for all films with more porous and less dense grains at higher Mn content. The increase in Mn doping ratio to $x = 0.1$ decreases the carrier density and the carrier type changes to the P-type conduction. The transmittance values increased with Mn doping whereas the reflectance decreased. The optical band gap increased from 0.25 to 0.39 eV. Two layer-model was successfully used to simulate the ellipsometry measurements. The main layer was described by a combined contribution of Drude and Lorentz models. The thickness, the optical constants, and the surface roughness of the undoped and Mn doped films were extracted from the ellipsometry measurements. Upon Mn doping, the PL was quenched.

1 Introduction

Bismuth Telluride (Bi_2Te_3) is one of the most important thermoelectric semiconductor materials which have been utilized in devices fabrication such as thermoelectric generators [1], flexible thermoelectric devices [2], thermoelectrics in sequencing reactions and driving DNA amplification [3], photodetector in

harsh working environments [4], thin film Hall bar device [5] and transducer for solar energy [6].

Doping of Bi_2Te_3 with transition metal is an active field of research due to the change in properties that can be tailored by the doping level and the numerous applications which can be utilized [7–10]. Mn doped Bi_2Te_3 films are no exception. One of the important effects is the layered crystal structure of Mn doped

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Structure Explication, Biological Evaluation, DNA Interaction, Electrochemistry and Antioxidant Activity of Iron (II) tri- and Tetra-Dentate Schiff base Amino Acid Complexes

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Received: 7 Jan. 2021, Revised: 2 Apr. 2021, Accepted: 17 Apr. 2021.

Published online: 1 May 2021

Abstract: New azomethine Schiff base amino acid ligands derived from the condensation reaction of 3-methoxysalicylaldehyde (MS) or 4-diethylaminosalicylaldehyde (DS) with some of α -amino acids (L-phenylalanine (Phe), L-histidine (His), DL-tryptophan (Trp)) and their Fe(II) complexes were prepared. Structures of the synthesized Fe(II) complexes were determined on the basis of elemental analysis, infrared, ultraviolet-visible spectra, thermal analysis and cyclic voltammetry (CV) as well as conductivity, magnetic susceptibility measurements. Moreover, the particle size distribution of the prepared complexes was determined by using transmittance electron microscope (TEM). The experimental results show that the investigated Fe(II) complexes contain hydrated water molecules (except DSPFe complex) and coordinated water molecules (only in MSHFe complex). The kinetic and thermal parameters were determined from the thermal data using Coast and Redfern method. The results suggest that MS or DS amino acid Schiff bases behave as monobasic tridentate ONO ligands and coordinate to Fe(II) in octahedral geometry according to the general formula $[\text{Fe}(\text{HL})_2] \cdot n\text{H}_2\text{O}$. But in the case of MSHFe complex, MSH ligand acts as tetradentate $(\text{NH}_4^+)[\text{Fe}(\text{HL})(\text{H}_2\text{O})\text{SO}_4] \cdot 2\text{H}_2\text{O}$. The conductivity values between $43.30\text{--}5.66 \Omega^{-1} \text{mol}^{-1} \text{cm}^{-2}$ in DMF suggest the presence of non-electrolyte species, except MSHFe complex is electrolyte species ($60.3 \Omega^{-1} \text{mol}^{-1} \text{cm}^{-2}$). Moreover, the antimicrobial evaluation of the prepared Schiff base amino acid ligands and their Fe(II) complexes was examined against three types of bacteria such as *B. subtilis* (+ve), *E. coli* (-ve) and *M. luteus* (+ve) and three types of fungi such as *A. niger*, *C. glabrata* and *S. cerevisiae*. The results of these studies signalizing that the metal chelates exhibit a stronger antimicrobial efficiency than their corresponding ligands. Moreover, the interaction of the prepared Fe(II) complexes with (CT-DNA) by using spectral studies, viscosity measurements and agarose gel electrophoresis was investigated. Furthermore, antioxidant activities of the synthesized complexes were examined by using the ABTS assay and showed that the prepared complexes have a good antioxidant activity.

Keywords: Amino acid, Fe(II) complexes, Antimicrobial, Cyclic voltammetry, antioxidant, DNA interaction.

1 Introduction

There are few amino acids which are principles for human beings such as: phenylalanine, tryptophan, and histidine. They are very much necessity, as they cannot be bio-synthesized by our body. Phenylalanine: Helps in boosting memory power and helps to maintain a healthy nervous system. Tryptophan: Plays a vital role in maintaining our appetite. Histidine: Helps in the yielding and synthesis of both RBC (red blood cells) and WBC (white blood cells).

Phenylalanine is important in the construction of

structural proteins in tissue. The concentrations of phenylalanine govern the amounts of other electrically neutral amino acids in the brain. Tryptophan catabolism in cancer is progressively more being identified as a marked microenvironmental factor that curbs antitumor immune responses. It has been suggested that the fundamental amino acid tryptophan is catabolized in the tumor tissue by the rate-restrictive enzyme indole amine-2, 3-dioxygenase (IDO) revealed in tumor cells or antigen-presenting cells [1]. Tryptophan is the only amino acid bound to plasma albumin [2]. Part of the tryptophan bound to albumin is available for uptake into the brain

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Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Study the effect of type of substrates on the microstructure and optical properties of CdTe Thin Films

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ARTICLE INFO

Keywords:

CdTe
thin films
microstructure
refractive index
optical energy gap

ABSTRACT

Cadmium telluride (CdTe) thin films are deposited on an ultrasonically cleaned substrate of different types by using thermal evaporation technique under pressure 2×10^{-5} mbar. The structural and morphological studies of all the films are accomplished using the X-ray diffraction method (XRD) and field emission scanning electron microscope (FE-SEM). CdTe found to have a polycrystalline structure. The grains were very uneven and the grain shape was irregular. A Jasco V-570 UV- visible - NIR spectrometer has been used to measure the optical properties in the range of wavelength from 200 to 2500 nm at normal incidence. The optical energy gap (E_g) is determined by using the Tauc's equation. The optical parameters such as; refractive index (n), static refractive index (n_0), infinite dielectric constant (ϵ_∞), dispersion energy (E_d), single oscillating energy (E_0), static dielectric constant (ϵ_s), free carrier concentration (N), plasma frequency (ω_p), relaxation time (τ), oscillator wavelength (λ_o), oscillator strength (S_0) and electronic polarizability (α_p) respectively are calculated. The optical measurements for CdTe films deposited on FTO substrate were properly used as absorber material for solar cell applications. Inversely, CdTe films deposited on a glass substrate is more suitable for a window in solar cell applications.

1. Introduction

In the latest years, Cadmium Telluride (CdTe) semiconductor is a compound with potential applications for using in photovoltaics of solar cells [1,2], optoelectronic devices such as detectors [3,4] and p-n junction devices [5]. It has Zinc blende crystal structure. CdTe is unique among II-VI compounds which make it important and quite suitable for several applicants as it may exhibit both n-type and p-types conductivity [6–8]. Otherwise, CdTe shows the p-type semiconductor because of the Cd vacancies rare present. CdTe is a direct band gap semiconductor and has an optimal width of the band gap of 1.5 eV, which is a suitable difference in the energy range for converting solar radiation into electricity [9,10]. So, CdTe thin films of thickness 1 μm found to have a high optical absorption coefficient and absorption of about 10^4 cm^{-1} , 92% respectively of the visible light [11]. This absorption value belongs to CdTe is better than that of crystalline silicon, which needs about 200 μm to reach the same value [12].

Several methods are used for the preparation of thin films of CdTe such as Sputtering [13,14], spray pyrolysis [3], close space vapor transport, metal-organic chemical vapor deposition and thermal evaporation [15–17]. Among the major advantages of thermal evaporation technique high deposition rates, relative simplicity, and low cost of the equipment must be mentioned. This process uses a strong vacuum environment, and so is capable of producing very high purity thin films [18–20].

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E-mail address: moh_f_2001@yahoo.com (M.F. Hasaneen).<https://doi.org/10.1016/j.ijleo.2020.165390>

Received 5 March 2020; Received in revised form 17 July 2020; Accepted 3 August 2020

Available online 7 August 2020

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Synergistic inhibition effect of novel counterion-coupled surfactant based on rice bran oil and halide ion on the C-steel corrosion in molar sulphuric acid: Experimental and computational approaches

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ARTICLE INFO

Article history:

Received 29 December 2020

Received in revised form 19 February 2021

Accepted 25 February 2021

Available online 27 February 2021

Keywords:

Counterion-coupled surfactant

Surface morphology

Synergism

Corrosion protection

Green synthesis

DFT

ABSTRACT

The counterion-coupled surfactant (RBOS-12) based on rice bran oil is synthesized, characterized, and evaluated as a new inhibitor for carbon steel corrosion. The inhibition, and synergistic effect performance of individual RBOS-12, and that is combined with chloride ions on the corrosion of carbon steel in a molar sulphuric acid medium at $30\text{--}60 \pm 1$ °C has been examined using open circuit potential-time, linear polarization resistance (LPR) corrosion rate, impedance spectroscopy (EIS), potentiodynamic polarization (PDP), surface topology (Field emission-scanning electron microscopy/Energy dispersive X-ray analysis (FE-SEM/EDS), X-ray diffraction (XRD) and UV-vis spectroscopic studies), density functional theory (DFT) and molecular dynamics (MD) simulations. Experimental findings exhibited that the inhibition capacity of individual RBOS-12 is 95.5% at the concentration of 1.0×10^{-3} M. Synergistic inhibition effect was observed between the RBOS-12 surfactant and the Cl⁻ ion additives, with the maximum corrosion inhibition capacity as high as ~99.1% at 1×10^{-5} M RBOS-12 + 0.1 M Cl⁻ ions. The individual RBOS-12 and RBOS-12/Cl⁻ system get adsorbed onto the metal interface through mixed categories of adsorption mainly with the chemisorption. Meanwhile, the adsorption mode follows the Langmuir isotherm model. FE-SEM/EDS and XRD investigates approve the protective and adsorption capabilities of the individual RBOS-12 and RBOS-12/Cl⁻ inhibitor systems. UV-vis spectroscopic analysis display that the additive interacts with metal in H₂SO₄ medium to form Fe-inhibitor complexes. DFT calculations and MD simulations further support the empirical outcomes. The findings exhibited that the prepared RBOS-12/Cl⁻ system can be used as economic, eco-friendly, and efficient corrosion inhibitor with good anticorrosion properties for metals in acidic environments.

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1. Introduction

Carbon steel (C-steel) has been considered as one of the most significant and usually utilized in innumerable engineering and manufacturing applications, including automotive, petroleum, water and power generation, chemical treating and a diversity of other manufacturing. The significance and extensive utilize of C-steel is related to its low-cost and outstanding mechanical-chemical characteristics [1,2]. Nevertheless, one of the major dilemmas of using C-steel is its susceptibility to corrosion in various corrosive solutions predominantly mineral acids for instance H₂SO₄ and HCl [3]. One of the efficient and essential tools to impede the C-steel corrosion in mineral acids is the application

of inhibitors, which diminishes the aggression of solutions towards C-steel surfaces [4].

Eco-friendly organic inhibitors applications are emerged to touch the environmental restrictions demands. So, inorganic inhibitors (such as phosphates, chromates, nitrates, and molybdates) that are extremely used in corrosion protection of metal/alloys (e.g., C-steel) are substituted despite their high capacity [5–8]. A survey of the previous studies on acid corrosion inhibitors indicates that most of the well-recognized additives contain N, S, and O atoms with N-containing carbon-based compounds as effective inhibitors in hydrochloric acid medium and those with S-containing compounds as effective inhibitors in sulphuric acid solution [9–13]. Compounds containing both N and S could deliver outstanding corrosion inhibition capacity compared with inhibitors containing either S or N [14,15]. The presence of larger electronegative atoms, like N and S, etc., in the inhibitor molecule is found to affect the inhibitor adsorption over corroding metal surface reinforcement efficient inhibition [16]. Organic surfactants, besides their eco-friendly and biodegradable properties they have excellent corrosion protection characteristics. They have high

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 Cite this: *RSC Adv.*, 2021, 11, 2905

Synthesis and antimicrobial activity of some novel 1,2-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidines bearing amino acid moiety†

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A new series of [1,2,4]-triazole bearing amino acid derivatives **2a–d–9a–d** were synthesized under green chemistry conditions *via* multicomponent reaction using lemon juice as an acidic catalyst. The obtained compounds were characterized by different spectral and elemental analyses. The obtained candidates showed promising antibacterial activity against some standard bacteria and multidrug resistant (MDR) clinical isolates. In contrast to the reference drugs cephalothin and chloramphenicol, the tested compounds showed substantial better MIC values towards the tested MDR strains. The most active compounds **3c**, **8a** and **9d** against MDR bacteria were tested for MBC and MIC index, the results indicated the bacteriostatic activity of these compounds. The most active compounds **2c**, **2d**, **3c**, **8a**, **8b**, **9a**, **9b**, **9c** and **9d** showed a high selectivity index towards antimicrobial activity against *K. pneumoniae* and *MRSA1* compared to mammalian cells, suggesting a good safety profile.

Received 24th September 2020

Accepted 29th December 2020

DOI: 10.1039/d0ra08189b

rsc.li/rsc-advances

1. Introduction

Facing emerging bacterial infections has become more challenging worldwide due to the increasing number of multidrug-resistant (MDR) microbes.^{1–7} This indicates the crucial need to develop new efficient anti-bacterial agents. Many factors contribute to mutations in microbial genomes leading to resistance to known antibiotics. For instance, it is broadly confirmed that the abuse of antibiotics can significantly increase the development of resistant-genotypes.^{8–10} As the number of infectious diseases and multidrug-resistant bacterial strains continues to increase, researchers are prompted to develop novel anti-microbial molecules.¹¹

From a medicinal chemistry prospective, creating new generation of therapeutic molecules with improved pharmacological properties and drug-tolerance profile, as well as fewer side effects, is an ultimate goal.¹² Hence, libraries with privileged heterocyclic scaffolds are frequently utilized in the development of new potent drugs.¹³ For instance, hybrids from 1,2,4-triazole derived compounds usually hold a series of pharmacological properties such as anticancer,^{14,15} antiviral,¹⁶ antitubercular,^{17,18} antifungal,¹⁹ antileishmanial²⁰ and antibacterial²¹ activities. However, only few reports about fused systems of 1,2,4-triazolo[1,5-*a*]pyrimidines were reported in literature with pronounced antibacterial activities.²² In addition, coupling with simple amino acids, *e.g.*, glycine and others, has been frequently attracted the interest of medicinal chemists due to its improving ability for the physicochemical and drug-likeness properties.^{20,23} In addition, glycine and its derivatives appear to be promising safe antimicrobial agents.^{24,25}

Being analogues of DNA purine bases, 1,2,4-triazolo[1,5-*a*]pyrimidines can be regarded as plausible substrates for enzymatic biochemical processes.²⁶ In particular, derivatives of [1,2,4]triazolo-[4,3-*a*]pyrimidines have recently been reported as potential antibacterials.^{27–30} It was reported that series of 1,2,4-triazolo[1,5-*a*]pyrimidines carboxamide derivatives attributed good narrow-spectrum antibacterial activity against *E. faecium* and possessed metabolic stability with low intrinsic clearance. Macromolecular synthesis assays revealed cell-wall biosynthesis as the target of these compounds.²² It is worth mentioning that recently, several 1,2,4-triazolo[1,5-*a*]pyrimidines were synthesized and screened for their antibacterial derivatives as DNA

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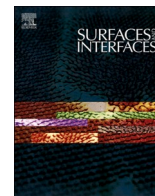
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† Electronic supplementary information (ESI) available. See DOI: 10.1039/d0ra08189b





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

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ARTICLE INFO

Keywords:

Polyazomethines
Inhibition
Surface morphology
Theoretical study
Acidic corrosion

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 thio-sulfurous [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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<https://doi.org/10.1016/j.surfin.2021.101037>

Received 27 December 2020; Received in revised form 28 January 2021; Accepted 17 February 2021

Available online 20 February 2021

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