3.4.5 Bibliometrics of the Publications during the last five years based on average Citation Index in Scopus/ Web of Science

Scopus Preview

Source details

Adalya

Scopus coverage years: 2009, from 2011 to 2014, from 2020 to 2023

Publisher: Suna Inan Kirac Akdeniz Medeniyetleri Aractirma Enstitusunun

ISSN: 1301-2746

Subject area: Arts and Humanities: History | Arts and Humanities: Conservation | Arts and Humanities: Archeology (arts and humanities) | Social Sciences: Archeology

Source type: Journal

CiteScore 2022 **0.1**

SJR 2022 **0.141**

SNIP 2022 **0.158**

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CiteScore 2022

$0.1 = \frac{\text{4 Citations 2019 - 2022}}{\text{28 Documents 2019 - 2022}}$

Calculated on 05 May, 2023

CiteScoreTracker 2023

$0.4 = \frac{\text{25 Citations to date}}{\text{68 Documents to date}}$

Last updated on 05 April, 2024 • Updated monthly

CiteScore rank 2022

Category	Rank	Percentile
Arts and Humanities — History	#1185/1599	25th
Arts and Humanities — Conservation	#84/102	18th
Arts and Humanities — Archeology (arts and	#316/368	14th

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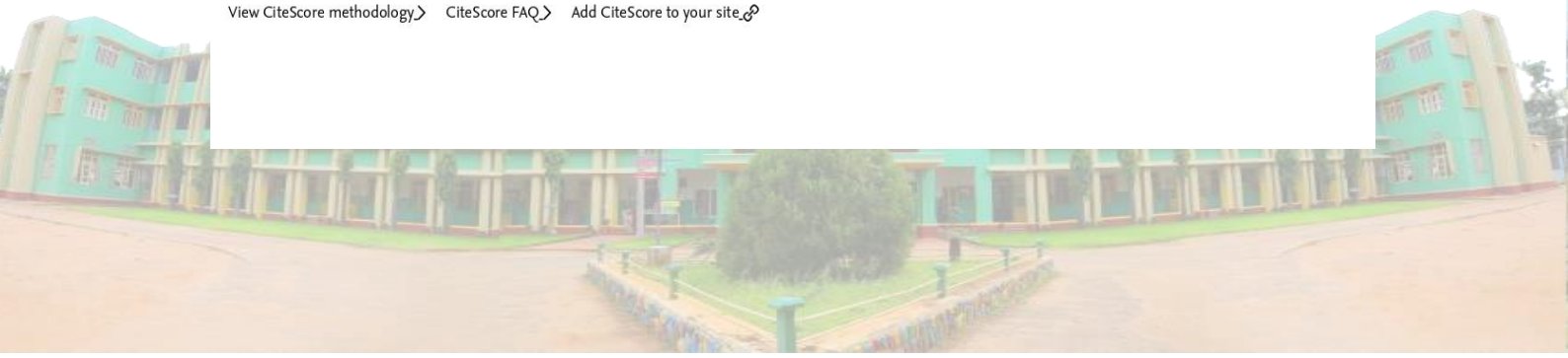

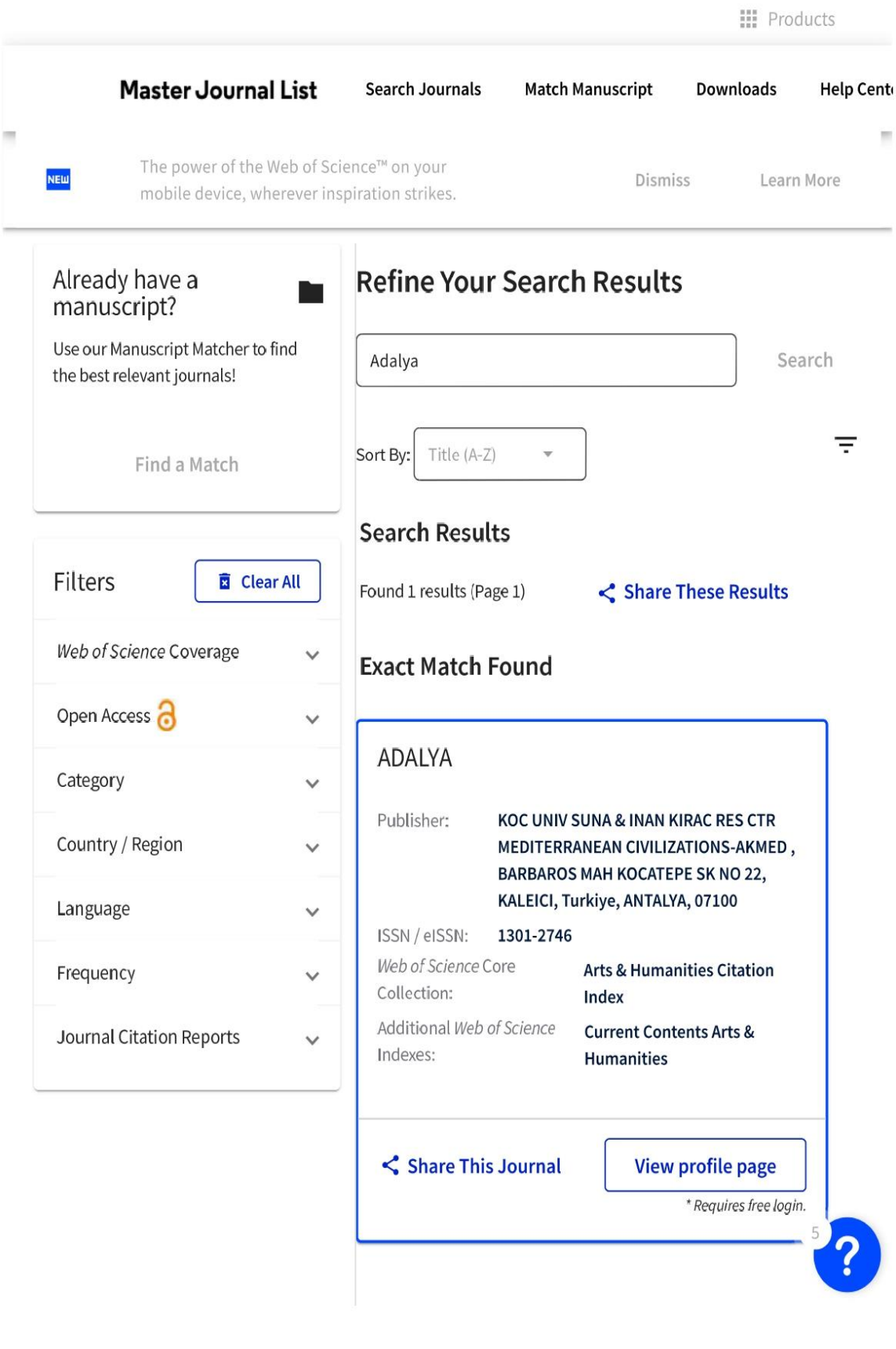
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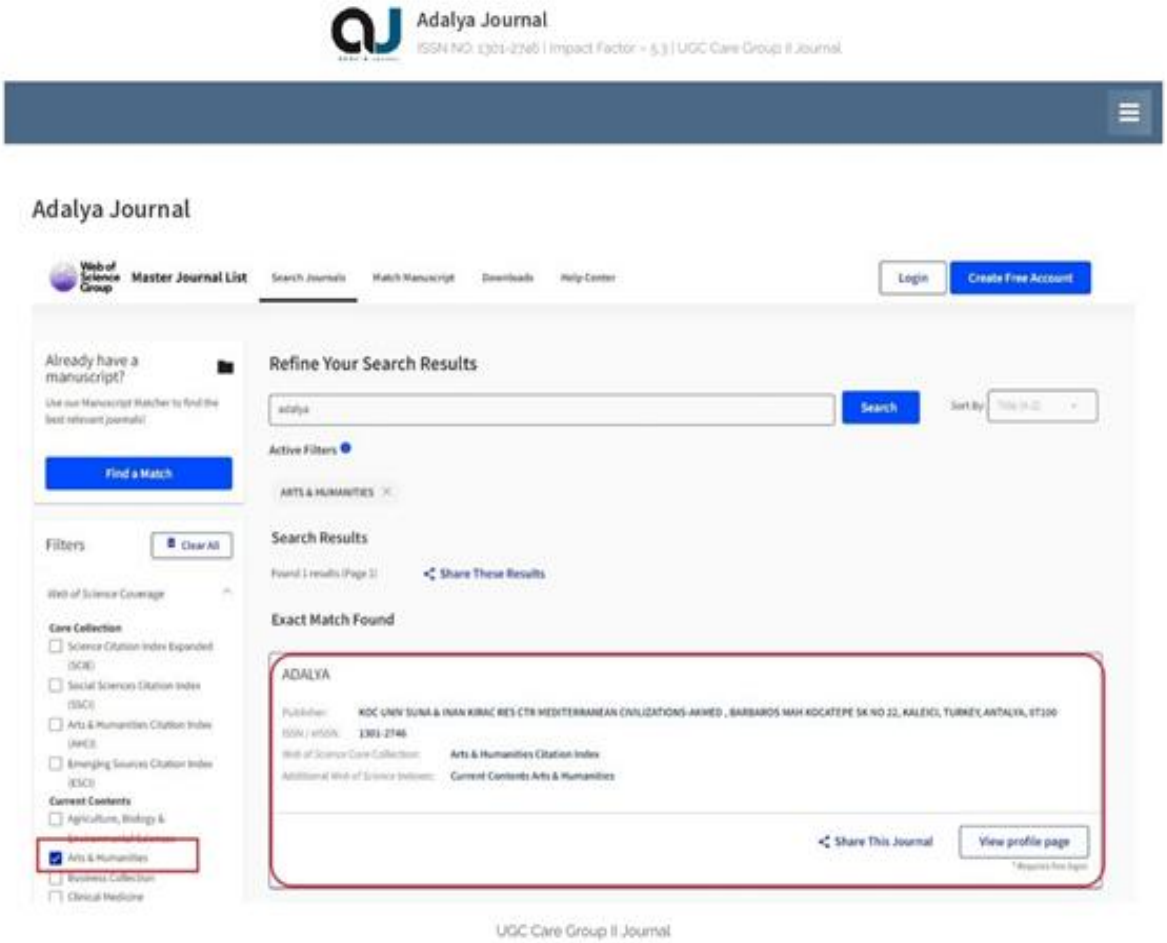

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THE MINIMUM DOMINATING ENERGY OF STAR RELATED GRAPHS

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[1]Research Scholar (19123042092002) , [2]Associate Professor & [3]Assistant Professor

[1] & [2] Holy Cross College (Autonomous), Nagercoil – 4, . &

[3]Malankara Catholic College, Mariagiri, Kaliyakkavilai,

[1], [2] & [3] Kanyakumari District, Tamilnadu, India.

Abstract : Chandrasekhar Adiga et.al., introduced the minimum covering energy of a graph which depends on its particular minimum cover. M.R. Rajesh Kanna et al defined the minimum dominating energy, $E_D(G)$ of some families of graphs such as, Star graph, Complete graph, Crown graph and Cocktail graphs. Motivated by this, we obtained the minimum dominating energy of star related graphs.

AMS Subject Classification: 05C50, 05C69

Keywords : minimum dominating set, minimum dominating matrix, minimum dominating eigenvalues, minimum dominating energy of a graph.

1. Introduction

Let G = (V,E) be a simple undirected graph. I. Gutman [3] introduced the concept of energy of a graph in the year 1978. Let G be a graph with n vertices and m edges and let the adjacency matrix of the graph be $R = (r_{ij})$. $\omega_1, \omega_2, \cdots, \omega_m$ assumed in non increasing order, are the eigenvalues of the graph G. The eigenvalues of G are real with sum equal to zero. Since, A is real symmetric. The energy $E(G)$ of G is defined to be the sum of the absolute values of the eigenvalues of G. i.e., $E(G) = \sum_{i=1}^{m} |\omega_i|$ [4,5]

2. The Minimum Dominating Energy

Definition 2.1: A **dominating set** in a graph G is a subset M of V(G) such that each element of V(G) – M is adjacent to at least one vertex of M.

Equivalently N[M] = V.

If M is a dominating set of a graph G, then every super set M' ⊃ M is also a dominating set.

Definition 2.2:[6] The **minimum dominating set** in a graph G is a dominating set of minimum cardinality. This set is also called γ - set.

Definition 2.3:[6]The **domination number** of G, denoted by γ(G), is the minimum cardinality of all dominating sets of G that is γ(G) = min { | M | / M ⊆ V, N[M] = V }

Definition 2.4:[6] Let G be a simple graph of order n with vertex set V = { $t_1, t_2, \ldots, t_m$ } and edge set E. Let M be a minimum dominating set of the graph G. The **minimum dominating matrix** of G is the m × m matrix defined by $R_{Md}(G) = (r_{ij})$, where

Scopus Preview

Source details

Journal of Mathematical and Computational Science

Scopus coverage years: from 2019 to 2021

(coverage discontinued in Scopus)

Publisher: SCIK Publishing Corporation

E-ISSN: 1927-5307

Subject area: Mathematics: General Mathematics | Computer Science: Computational Theory and Mathematics

Source type: Journal

CiteScore 2020
0.2

SJR 2020
0.120

SNIP 2022
0.499

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Calculated on 05 May, 2021

CiteScore rank 2020

Category	Rank	Percentile
Mathematics — General Mathematics	#362/378	4th
Computer Science — Computational Theory and Mathematics	#131/133	1st

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The authors declare that there is no conflict of interests.

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Quantitative analysis of transmission dynamic of Boko Haram

Available online at http://scik.org
J. Math. Comput. Sci. 11 (2021), No. 5, 6007-6017
https://doi.org/10.28919/jmcs/6225
ISSN: 1927-5307

THE MONOPHONIC GLOBAL DOMINATION NUMBER OF A GRAPH

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Affiliated to Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli-627 012, Tamil Nadu, India

Abstract. A set $M \subseteq V$ is said to be a monophonic global dominating set of G if M is both a monophonic set and a global dominating set of G. The minimum cardinality of a monophonic global dominating set of G is the monophonic global domination number of G and is denoted by $\overline{\gamma}_m(G)$. A monophonic global dominating set of cardinality $\overline{\gamma}_m(G)$ is called a $\overline{\gamma}_m$-*set* of G. The monophonic global domination number of certain classes of graphs are determined. It is proved that $2 \leq \overline{\gamma}_m(G) \leq \overline{\gamma}_g(G) \leq n$, where $\overline{\gamma}_g(G)$ is a geodetic global domination number of a G. It is shown that for every pair of positive integers a and b with $2 \leq a \leq b$, there exists a connected graph G such that $\overline{\gamma}_m(G) = a$ and $\overline{\gamma}_g(G) = b$.

Keywords: monophonic global domination number; global domination number; monophonic number; domination number.

2010 AMS Subject Classification: 05C38, 05C69, 05C12.

1. INTRODUCTION

By a graph $G = (V, E)$, we mean a finite,undirected connected graph without loops or multiple edges. The *order* and *size* of G are denoted by m and n respectively. For basic graph theoretic terminology, we refer to [2]. Two vertices u and v are said to be *adjacent* if uv is

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†Research Scholar, Register Number: 20123042092008

Received June 05, 2021

Scopus Preview

Source details

Design Engineering (Toronto)

Scopus coverage years: from 1971 to 1976, from 1996 to 2005, from 2012 to Present

Publisher: Rogers Media Publishing

ISSN: 0011-9342

Subject area: Engineering: General Engineering

Source type: Trade Journal

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CiteScore 2022
0.0

SJR 2022
0.101

SNIP 2017
0.000

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CiteScore 2022

0.0 = 0 Citations 2019 - 2022 / 30 Documents 2019 - 2022

Calculated on 05 May, 2023

CiteScoreTracker 2023

0.0 = 0 Citations to date / 31 Documents to date

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CiteScore rank 2022

Category	Rank	Percentile
Engineering └ General Engineering	#301/302	0th

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Design Engineering (Toronto)

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SCOPUS classifier

1708 Hardware and Architecture
2200 Engineering(all)
2210 Mechanical Engineering

ISSN: 00119342

The scientific journal is included in the Scopus database.

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00137758	Engineer	SJR: 0.1
10763333	Resource: Engineering and Technolog...	SJR: 0.102
23492473	Journal of Engineering Education Tran...	SJR: 0.114

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The Minimum Dominating Seidel Energy of Some Graphs

V. M. Arul Flower Mary, Victoria Jayafin Nisha S L, M. Regees

Keywords: minimum dominating set, minimum dominating seidel matrix, minimum dominating seidel eigenvalues, minimum dominating seidel energy of a graph.

ABSTRACT

M.R. Rajesh Kanna et al defined the minimum dominating seidel energy, $E_{Sd}(G)$ of some families of graphs such as, Star graph, Complete graph, Crown graph and Cocktail graphs. Motivated by this, we obtained the minimum dominating seidel energy of Book graph and Friendship graphs. Relation between domination number, energy and rank of minimum dominating seidel matrix of graphs are also established.

Scopus Preview

Source details

Proyecciones

Scopus coverage years: from 2000 to 2002, from 2006 to Present

Publisher: Universidad Catolica del Norte

ISSN: 0716-0917 E-ISSN: 0717-6279

Subject area: Mathematics: General Mathematics

Source type: Journal

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CiteScore 2022
1.1

SJR 2022
0.320

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0.786

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Last updated on 08 November, 2023 • Updated monthly

CiteScore rank 2022

Category	Rank	Percentile
Mathematics — General Mathematics	#237/387	38th

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ISSN 0717-6279 (On line)

The edge-to-edge geodetic domination number of a graph

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Received: 28 March 2020 | Accepted: 12 January 2021

Abstract:

Let $G = (V, E)$ be a connected graph with at least three vertices. A set $S \subseteq E(G)$ is called an edge-to-edge geodetic dominating set of G if S is both an edge-to-edge geodetic set of G and an edge dominating set of G. The edge-to-edge geodetic domination number $\gamma_{gee}(G)$ of G is the minimum cardinality of its edge-to-edge geodetic dominating sets. Some general properties satisfied by this concept are studied. Connected graphs of size m with edge-to-edge geodetic domination number 2 or m or $m-1$ are characterized. We proved that if G is a connected graph of size $m \geq 4$ and $\bar{G}$ is also connected, then $4 \leq \gamma_{gee}(G) + \gamma_{gee}(\bar{G}) \leq 2m - 2$. Moreover we characterized graphs for which the lower and the upper bounds are sharp. It is shown that, for every pair of positive integers a, b with $2 \leq a \leq b$, there exists a connected graph G with $g_{ee}(G) = a$ and $\gamma_{gee}(G) = b$. Also it is shown that, for every pair of positive integers a and b with $2 < a \leq b$, there exists a connected graph G with $\gamma_e(G) = a$ and $\gamma_{gee}(G) = b$, where $\gamma_e(G)$ is the edge domination number of G and $g_{ee}(G)$ is the edge-to-edge geodetic number of G.

Keywords: Edge-to-edge geodetic domination number; Edge-to-edge geodetic number; Edge domination number; Domination number; Geodetic number

MSC (2020): 05C69, 05C12.

Cite this article as (IEEE citation style):

J. John and V. Sujin Flower, "The edge-to-edge geodetic domination number of a graph", *Proyecciones (Antofagasta, On line)*, vol. 40, no. 3, pp. 635-658, 2021, doi: 10.22199/issn.0717-6279-4057

Scopus Preview

Source details

South East Asian Journal of Mathematics and Mathematical Sciences

Scopus coverage years: from 2019 to 2023

Publisher: RAMANUJAN SOCIETY OF MATHEMATICS AND MATHEMATICAL SCIENCES

ISSN: 0972-7752 E-ISSN: 2582-0850

Subject area: Mathematics: Algebra and Number Theory | Mathematics: Applied Mathematics | Mathematics: Analysis | Mathematics: Discrete Mathematics and Combinatorics | Mathematics: Computational Mathematics

Source type: Journal

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SJR 2022
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SNIP 2022
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CiteScoreTracker 2023

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Last updated on 05 April, 2024 • Updated monthly

CiteScore rank 2022

Category	Rank	Percentile
Mathematics — Algebra and Number Theory	#114/117	2nd
Mathematics — Applied Mathematics	#597/609	2nd
Mathematics		

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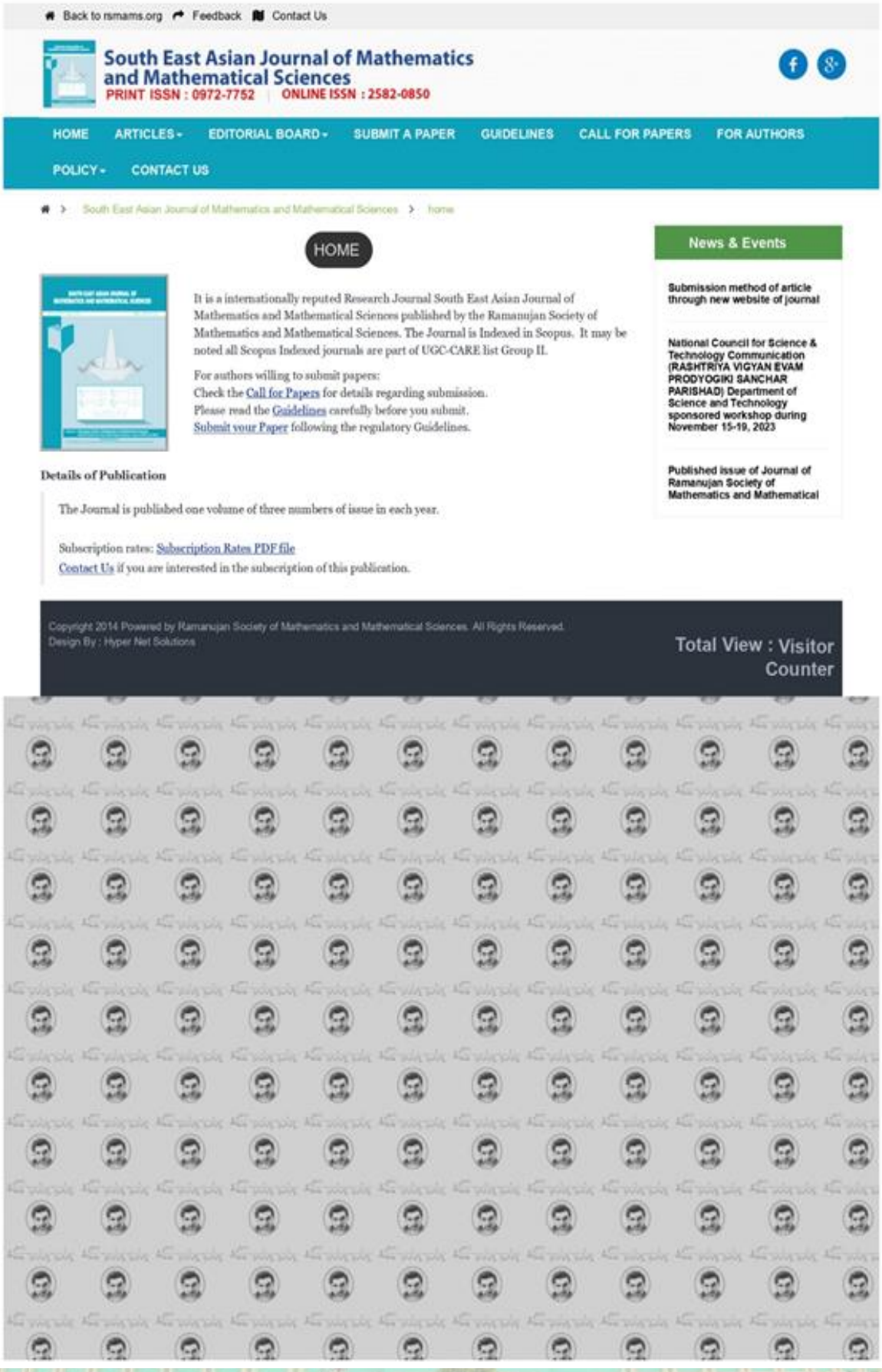

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ISSN (Print): 0972-7752

THE CONNECTED GEODETIC VERTEX COVERING NUMBER OF A GRAPH

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(**Received:** *Mar. 18, 2020* **Accepted:** *Jan. 02, 2021* **Published:** *Apr. 30, 2021*)

Abstract: For a connected graph G of order $n \geq 2$, a set $S \subseteq V(G)$ is a *geodetic vertex cover* of G if S is both a geodetic set and a vertex cover of G. The minimum cardinality of a geodetic vertex cover of G is defined as the *geodetic vertex covering number* of G and is denoted by $g_a(G)$. Any geodetic vertex cover of cardinality $g_a(G)$ is a g_a- set of G. A *connected geodetic vertex cover* of G is a geodetic vertex cover S such that the subgraph $G[S]$ induced by S is connected. The minimum cardinality of a connected geodetic vertex cover of G is the *connected geodetic vertex covering number* of G and is denoted by $g_{ac}(G)$. A connected geodetic vertex cover of cardinality $g_{ac}(G)$ is called a g_{ac} - set of G. Some general properties satisfied by connected geodetic vertex covering sets are studied. The connected geodetic

Scopus Preview

Source details

Proyecciones

Scopus coverage years: from 2000 to 2002, from 2006 to Present

Publisher: Universidad Catolica del Norte

ISSN: 0716-0917 E-ISSN: 0717-6279

Subject area: Mathematics: General Mathematics

Source type: Journal

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$$1.1 = \frac{385 \text{ Citations to date}}{354 \text{ Documents to date}}$$

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PDF

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Vol. 40, N° 5, pp. 1097-1116, October 2021.
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10.22199/issn.0717-6279-4258

k-super cube root cube mean labeling of graphs

V. Princy Kala
Holy Cross College (Autonomous), India
Received : June 2020. Accepted : January 2021

Abstract

Consider a graph G with $|V(G)| = p$ and $|E(G)| = q$ and let $f : V(G) \to \{k, k+1, k+2, \ldots p+q+k-1\}$ be an injective function. The induced edge labeling f^* for a vertex labeling f is defined by $f^*(e) = \left\lfloor \sqrt[3]{\frac{f(u)^3+f(v)^3}{2}} \right\rfloor$ or $\left\lceil \sqrt[3]{\frac{f(u)^3+f(v)^3}{2}} \right\rceil$ for all $e = uv \in E(G)$ is bijective. If $f(V(G)) \cup \{f^*(e) : e \in E(G)\} = \{k, k+1, k+2, \ldots, p+q+k-1\}$, then f is called a k-super cube root cube mean labeling. If such labeling exists, then G is a k-super cube root cube mean graph. In this paper, I introduce k-super cube root cube mean labeling and prove the existence of this labeling to the graphs viz., triangular snake graph T_n, double triangular snake graph $D(T_n)$, Quadrilateral snake graph Q_n, double quadrilateral snake graph $D(Q_n)$, alternate triangular snake graph $A(T_n)$, alternate double triangular snake graph $AD(T_n)$, alternate quadrilateral snake graph $A(Q_n)$, & alternate double quadrilateral snake graph $AD(Q_n)$.

Keywords: *k-super cube root cube mean labeling, k-super cube root cube mean graph, snake graph, alternate snake graph.*

MSC(2020): *05C78.*

Scopus Preview

Source details

Journal of Mathematical and Computational Science

Scopus coverage years: from 2019 to 2021
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E-ISSN: 1927-5307
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Source type: Journal

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All authors have read the manuscript and agree to publish it.

The authors declare that there is no conflict of interests.

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ISSN: 1927-5307

THE EDGE GEODETIC VERTEX COVERING NUMBER OF A GRAPH

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Abstract. For a connected graph G of order $n \geq 2$, a set $S \subseteq V(G)$ is an *edge geodetic vertex cover* of G if S is both an edge geodetic set and a vertex covering set of G. The minimum cardinality of an edge geodetic vertex cover of G is defined as the *edge geodetic vertex covering number* of G and is denoted by $g_{1a}(G)$. Any edge geodetic vertex cover of cardinality $g_{1a}(G)$ is a g_{1a} - set of G. Some general properties satisfied by edge geodetic vertex cover are studied. The edge geodetic vertex covering number of several classes of graphs are determined. Connected graphs of order n with edge geodetic vertex covering number 2 is characterized. A few realization results are given for the parameter $g_{1a}(G)$.

Keywords: geodesic; edge geodetic set; vertex covering set; edge geodetic vertex cover; edge geodetic vertex covering number.

2010 AMS Subject Classification: 05C12.

1. INTRODUCTION

By a graph $G = (V, E)$, we mean a finite undirected connected graph without loops and multiple edges. The *order* and *size* of G are denoted by n and m, respectively. For basic graph

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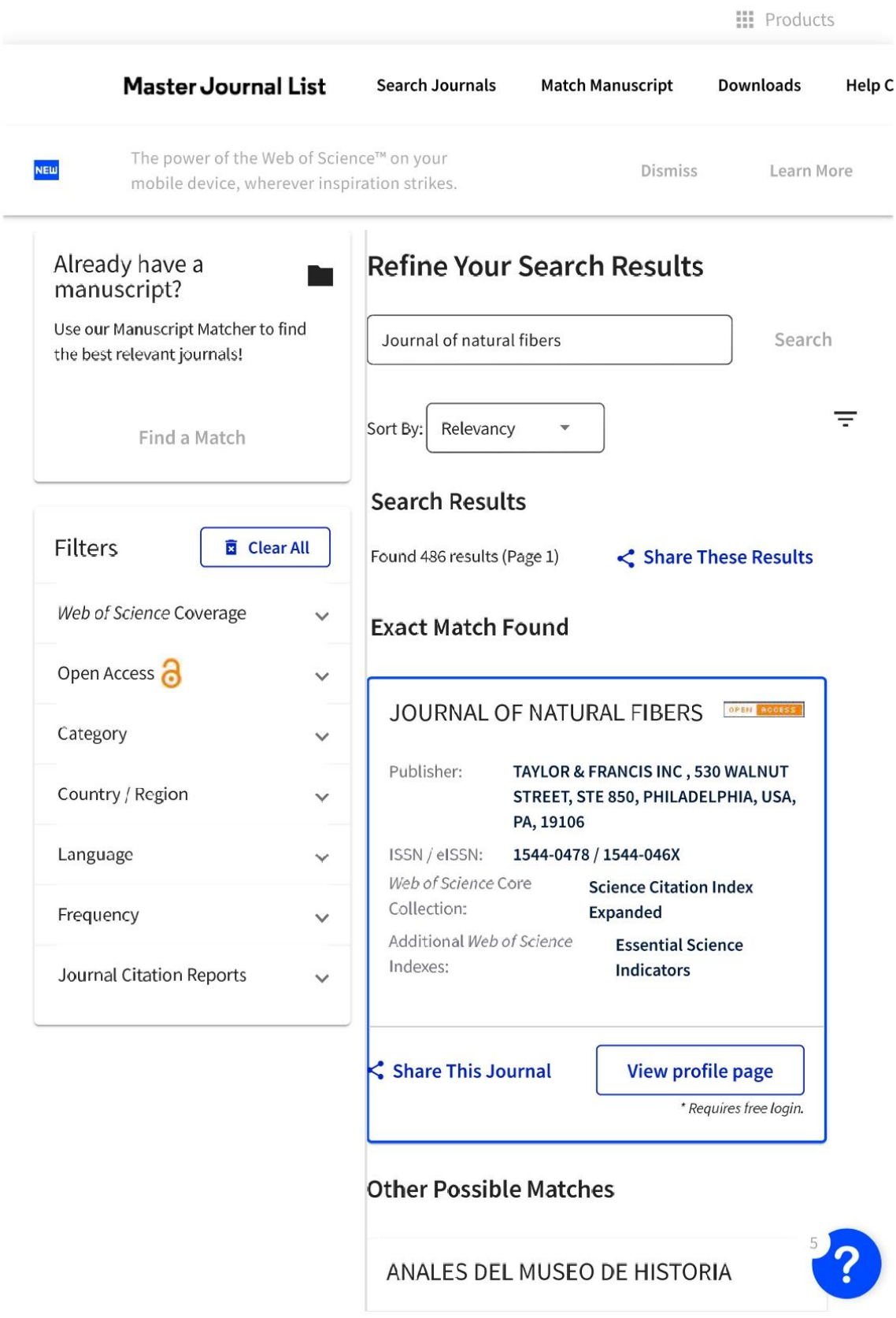
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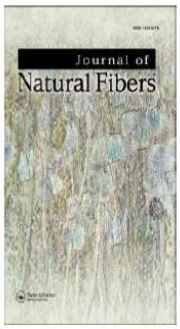

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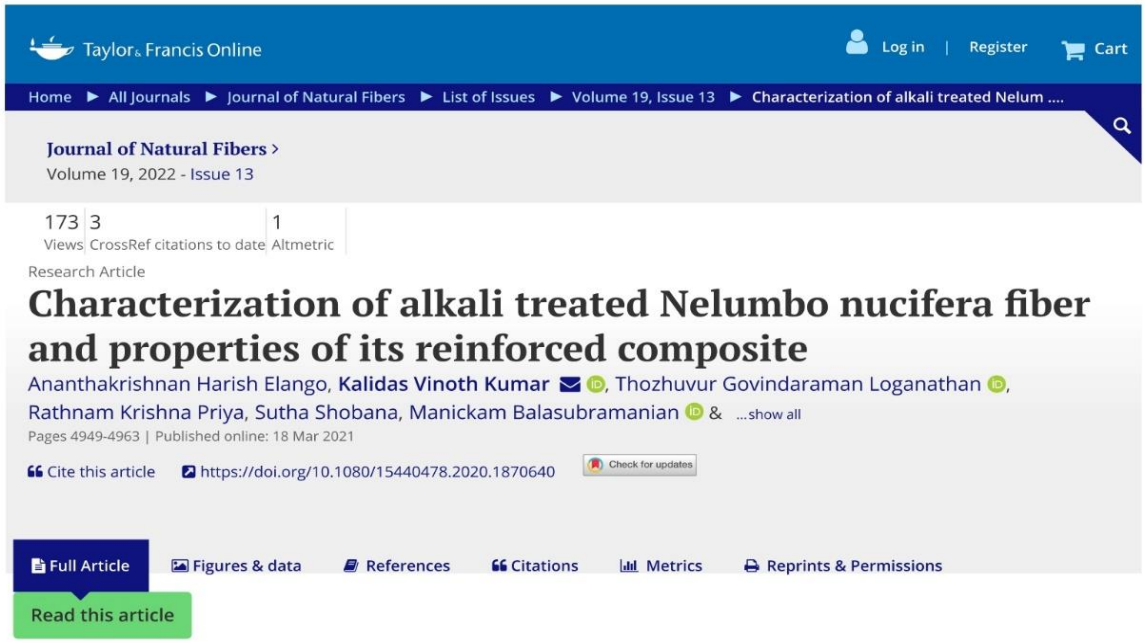


ABSTRACT

Natural fibers are being extensively used in recent technological and structural applications due to the need for biodegradable materials. This paper deals with extraction of new cellulosic fiber from the stem of *Nelumbo nucifera* (*Nn*) (lotus) and the investigations *via* physical, structural and thermal properties on the alkali-treated fiber were carried out. The XRD analysis of the *Nn* fiber provides the crystallinity index of about 52.53% that implies its high crystalline structure and own associated strength. The FTIR analysis proves the presence of alcoholic and alpha keto carboxylic acid in *Nn* fiber. Thermal stability of *Nn* composite is found around 210°C and the TGA results prove that the extracted as well as alkali-treated fibers provide a good reinforcement to the matrix, which can be well synthesized mechanically improved biocomposites. Test samples of three different weight % of *Nn* fiber with the epoxy basement are designated as L10, L15 and L20 to measure the tensile and flexural strength. Test sample with L20 as weight % exhibits better Young's and flexural modulus. Alkali treated *Nn* composite is an important candidate for the natural fiber reinforcement and such a category can serve as a good material for household applications.

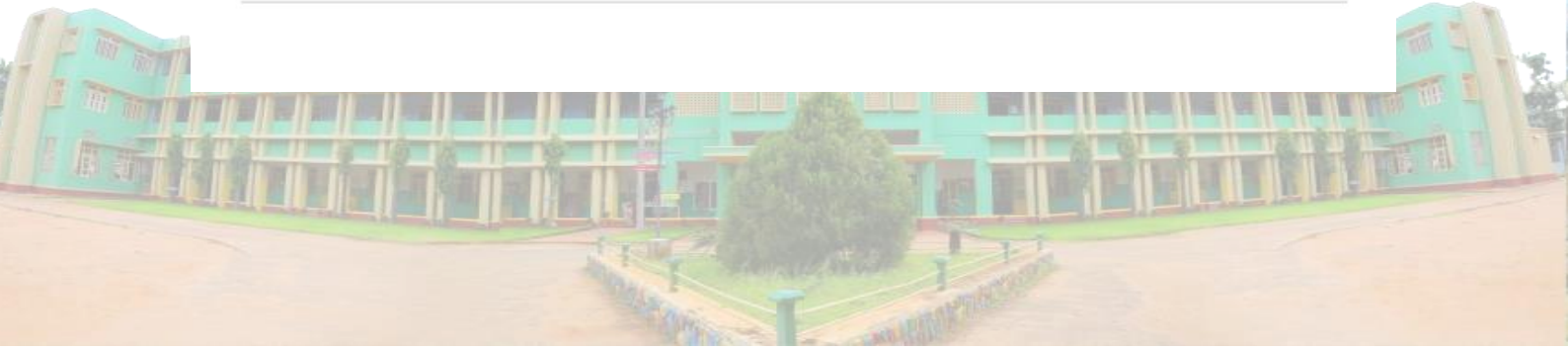
抽象:

由于需要生物降解材料，天然纤维正广泛应用于最近的技术和结构应用. 本文论述了从Nelumbo nucifera（Nn）（莲花）茎中提取新的纤维素纤维，并进行了碱处理纤维的物理、结构和热特性的研究. Nn纤维的XRD分析提供约52.53%的结晶指数，这意味着其高晶体结构和自身相关强度. FTIR 分析证明 Nn 纤维中存在酒精和α酮碳氧酸. Nn复合材料的热稳定性在210oC左右，TGA结果表明，提取的和碱处理的纤维对基体提供了很好的强化，可以很好地合成机械改进的生物复合材料. 使用环氧基底的 Nn 纤维三个不同重量 % 的测试样品被指定为 L10、L15 和 L20，用于测量拉伸和弯曲强度. 以L20为重量的试验样品表现出更好的杨和弹性模量. 碱处理Nn复合材料是天然纤维增强的重要候选材料，此类产品可作为家庭应用的好材料.

KEYWORDS: Nelumbo nucifera fiber | powder XRD | ftir | thermal | crystallinity index | mechanical properties | 关键字:纤维 | *powder XRD* | 粉末 | 热 | 结晶指数 | 机械性能

Correction Statement

This article has been republished with minor changes. These changes do not impact the academic content of the article.



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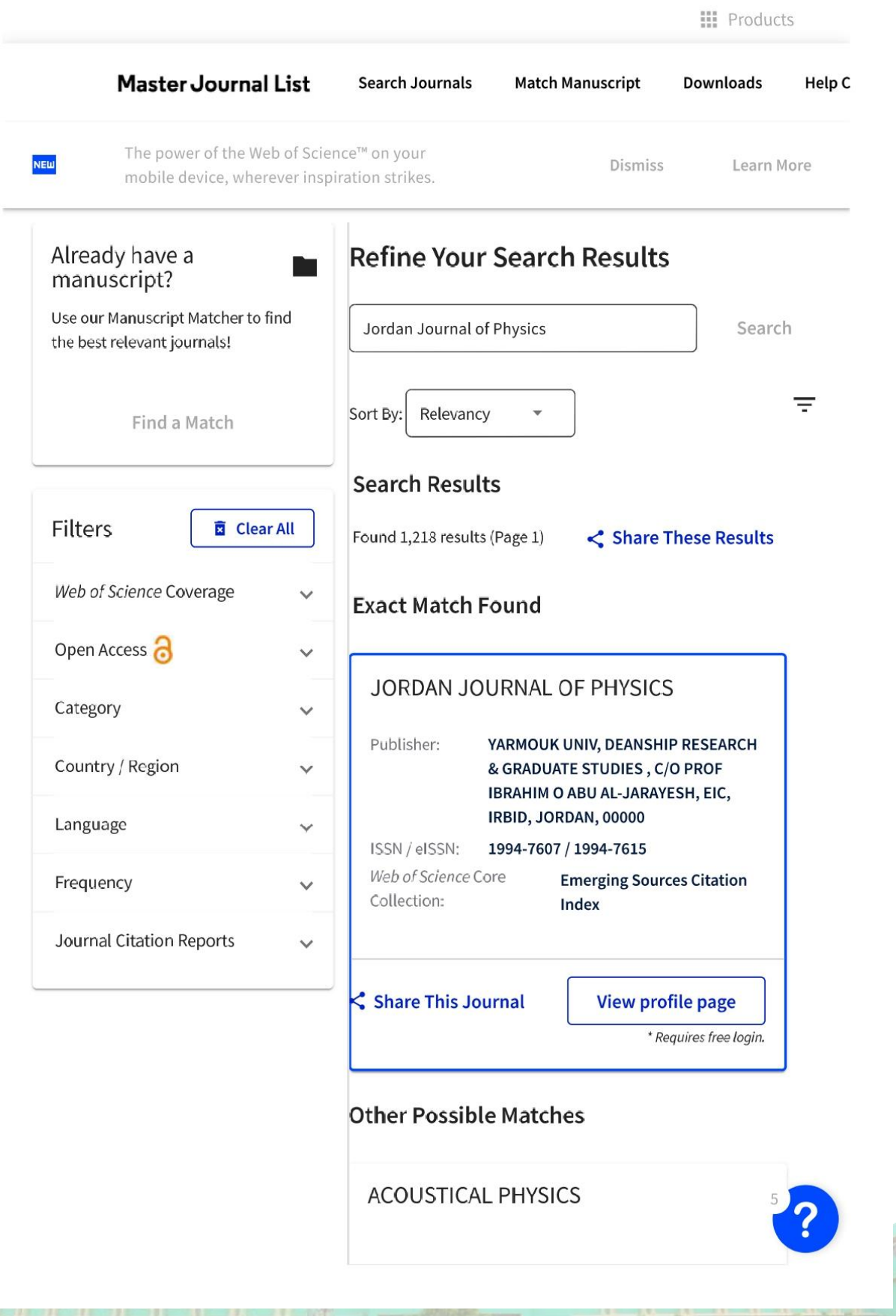
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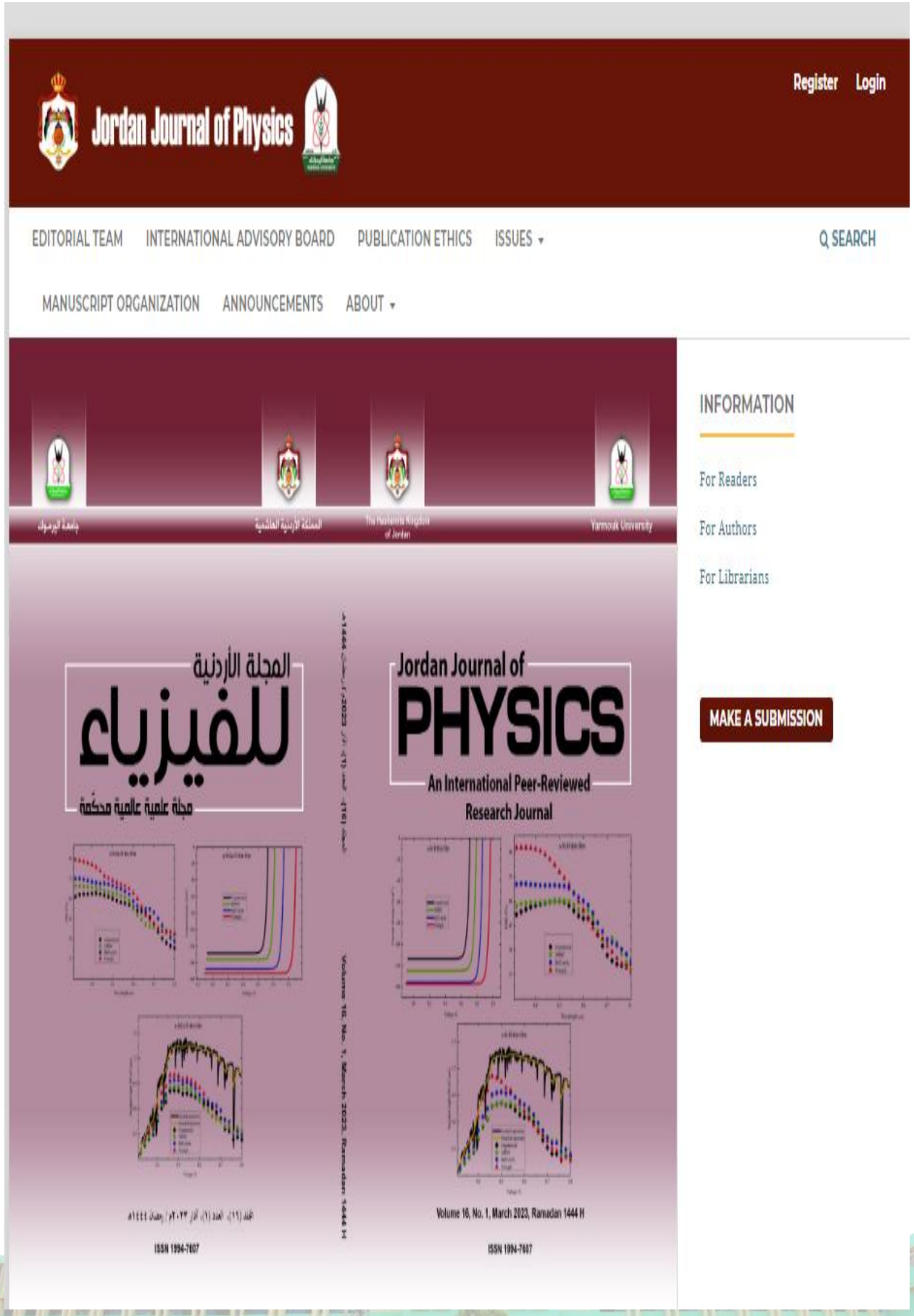
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Volume 14, Number 5, 2021. pp. 419-424

Jordan Journal of Physics

ARTICLE

Structural and Surface Characteristics of CuO and Pt/CuO Nanostructured Thin Films

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Doi:

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Abstract: The most prominent and utilizable platinum-coated copper Oxide nanostructured thin films are prepared using the SILAR method. Their structural properties have been studied using X-ray diffraction (XRD) and Raman spectroscopy. XRD pattern reveals the phase purity and crystallinity of CuO nanostructures. The average grain size estimated from XRD gives diameters in the range of 14 - 27 nm. Raman spectra explain the structural information of CuO and Pt/CuO nanostructured thin films, in which the peaks observed at 328 cm^{-1}, 609.32 cm^{-1} and 1141.77 cm^{-1} are the different phonon modes of CuO. The peak at 2136 cm^{-1} provides strong evidence for the formation of platinum on CuO nanostructures. The SEM micrograph confirms the floral morphology, which is composed of nano petals. From the observed morphology, it is observed that the deposited thin films such as CuO and Pt/CuO will give interesting applications to our society by being self-cleaning agents, photocatalysts, semiconductor devices, optical fibers, … etc.

Keywords: CuO, Pt/CuO, Structural analysis, SILAR, Crystallinity.

1. Introduction

Copper oxide, including cuprous oxide (copper (I) oxide) and cupric oxide (copper (II) oxide), is formed when copper is exposed to oxygen [1]. These semiconductor oxides have been investigated for various purposes, such as the inherent abundance of starting material (Cu), the ease of production by Cu oxidation, their non-toxic nature and the reasonably good electrical and optical properties exhibited by CuO [2]. Previous works showed that many of the growth methods for copper oxide resulted in a combined growth of copper (I) oxide (Cu_2O) and copper (II) oxide (CuO). However, CuO is a more widely used material than Cu_2O due to its stability. Cupric oxide (CuO) possesses a monoclinic crystal structure with a bandgap of 1.22–2.0 eV [3, 4]. Its high optical absorption coefficient in the visible range and reasonably good electrical properties constitute important advantages and render CuO as the most

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Scopus Preview

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Scopus coverage years: from 1990 to Present

Publisher: Springer Nature

ISSN: 0957-4522 E-ISSN: 1573-482X

Subject area: Engineering: Electrical and Electronic Engineering | Physics and Astronomy: Condensed Matter Physics | Physics and Astronomy: Atomic and Molecular Physics, and Optics | Materials Science: Electronic, Optical and Magnetic Materials

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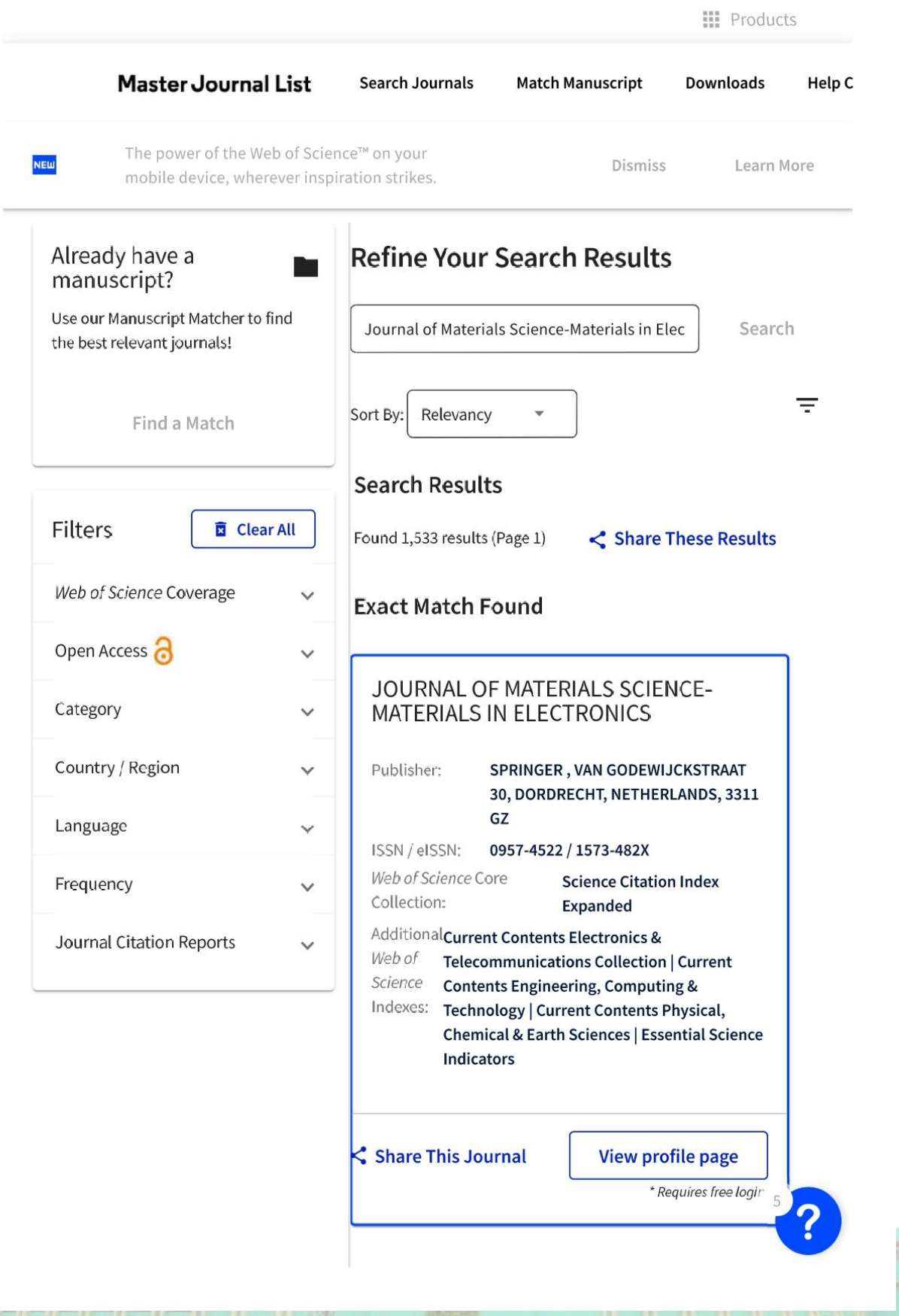
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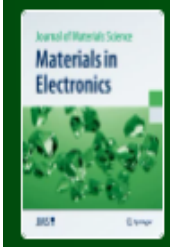

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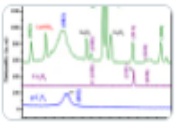

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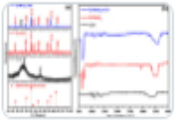

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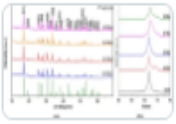

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Surface-enhanced Raman spectroscopy studies of orderly arranged silica nanospheres-synthesis, characterization and dye detection

| Published: 29 September 2021

| Volume 32, pages 26596–26607, (2021) Cite this article

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M. Ramuthai, Shaik Habibuddin, S. Sonia, Naidu Dhanpal Jayram, K. Deva Arun Kumar, Mohd. Shkir, H. Algarni & S. AlFaify

Abstract

Silica nanospheres have been explored much for drug delivery, photocatalysis, sensors and energy storage applications. It also acts as a template for Surface-Enhanced Raman Spectroscopy (SERS) substrates. Uniform nanostructures at low cost with high reproducibility are the major challenges in SERS substrate fabrication. In the present work, silica nanospheres were synthesized using stober method and deposited on to glass slides using Vertical deposition techniques. Different size/thickness of Silver (Ag) nanoparticles were deposited onto silica thin films using sputter deposition technique. The monodispersity of silica nanospheres and size of silver nanoparticles (10 nm, 20 nm and 30 nm) were confirmed by FESEM analysis. The structural properties were confirmed through XRD. UV–Vis analysis revealed that the plasmonic properties of $Ag@SiO_2$ give high surface plasmons for 30 nm thickness of silver. The binding energy of $Ag@SiO_2$ confirmed through XPS spectrum. The fabricated SERS substrates were used to detect Rhodamine 6G (R6G), Methylene blue (MB), Methylene violet (MV) and Methyl orange dyes as an analyte molecule with a limit of detection at about 10^{-11} mol/L. The addition of SiO_2 nanospheres decreases the Ag oxidation rate and increases their stability. The maximum enhancement factor (1.5×10^7) achieved for 30nm thickness of $Ag@SiO_2$. The results and technique establish the potential applications and reproducible SERS substrate.

Scopus Preview

Source details

Journal of Materials Science: Materials in Electronics

Scopus coverage years: from 1990 to Present

Publisher: Springer Nature

ISSN: 0957-4522 E-ISSN: 1573-482X

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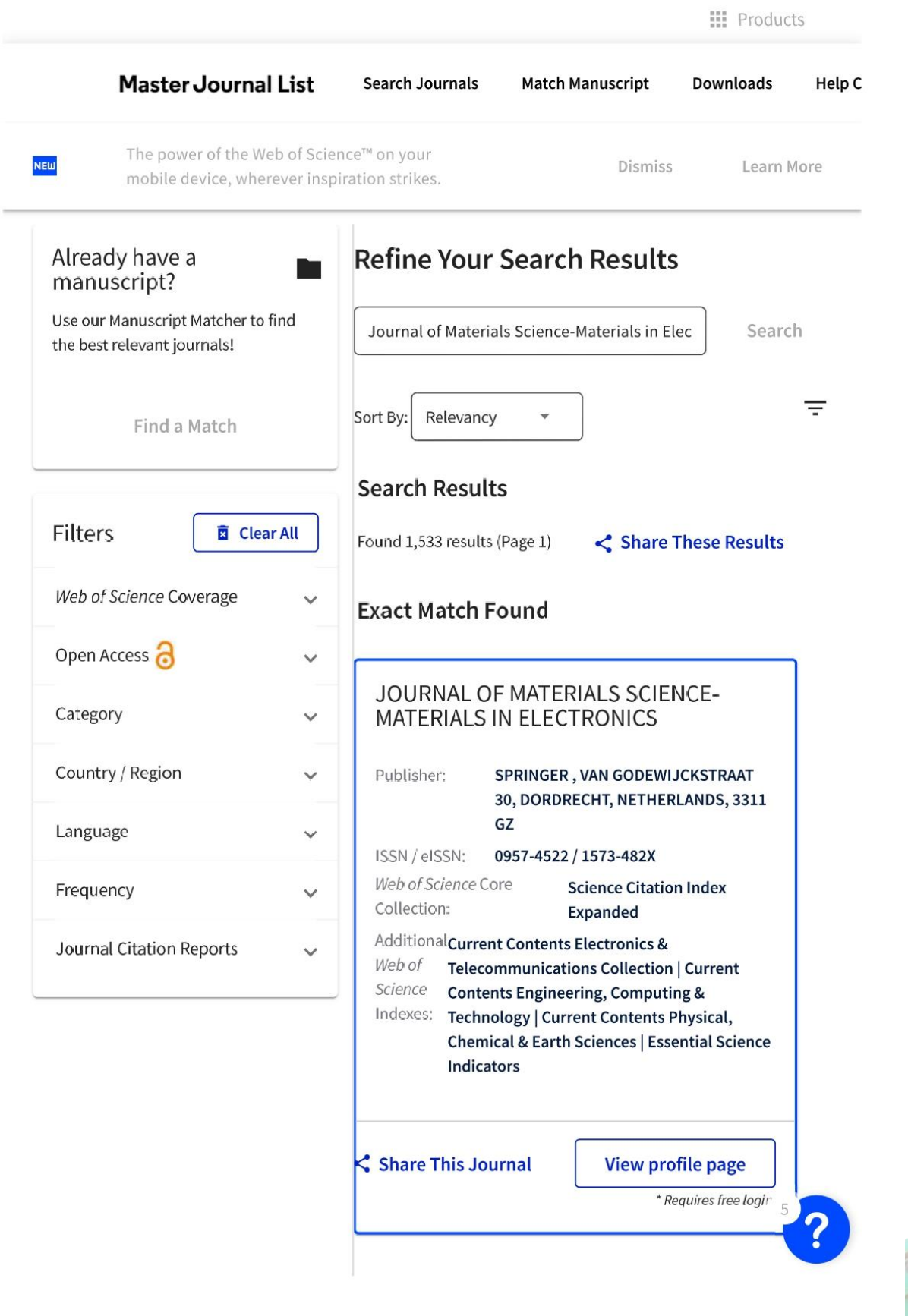
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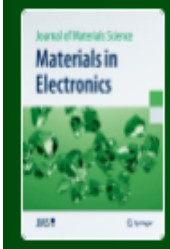

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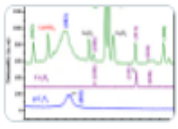

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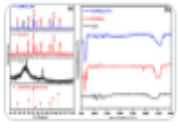
Facile synthesis of perovskite $ZnMnO_3$ composite with reduced graphene oxide via solvothermal route for supercapacitor applications



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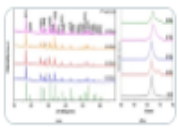

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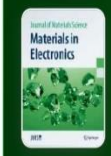
Enhanced linear and non-linear optical activity of lead onto L-threonine cadmium acetate crystal

| Published: 02 May 2021

| Volume 32, pages 13261–13268, (2021) Cite this article



M. Abila Jeba Queen ✉, K. C. Bright, S. Mary Delphine & P. Aji Udhaya

Abstract

Herein, we describe the growth and characterization of new crystal lead-doped L-threonine cadmium acetate (LTCA). The supramolecular coordination compounds are crystallized by slow evaporation technique at ambient temperature. The X-ray diffraction techniques confirm monoclinic crystal system. The presence of lead and the LTCA lattices were identified using EDAX analysis. L-Threonine amino acids have unique properties like zwitterionic nature and molecular chirality, which improve the optical properties of the lead-doped crystal. The linear optical parameters such as optical band gap and refractive indexes are estimated at lower cutoff wavelength from UV–Vis analysis. The variation of dielectric constant, dielectric loss with frequency is studied using LCR meter. Due to the electropositive character of lead the static permittivity increases. Magnetic behavior changes to paramagnetic nature due to the inclusion of lead. TG/DTA analysis suggests that the crystal is thermally stable up to 135.32 °C. Using Nd-YAG laser, the NLO property was studied and the lead-doped LTCA crystal shows higher SHG efficiency than the LTCA crystal.

Scopus Preview

Source details

Phosphorus, Sulfur and Silicon and the Related Elements

Scopus coverage years: from 1989 to Present

Publisher: Taylor & Francis

ISSN: 1042-6507 E-ISSN: 1563-5325

Subject area: Chemistry: Inorganic Chemistry | Chemistry: Organic Chemistry | Biochemistry, Genetics and Molecular Biology: Biochemistry

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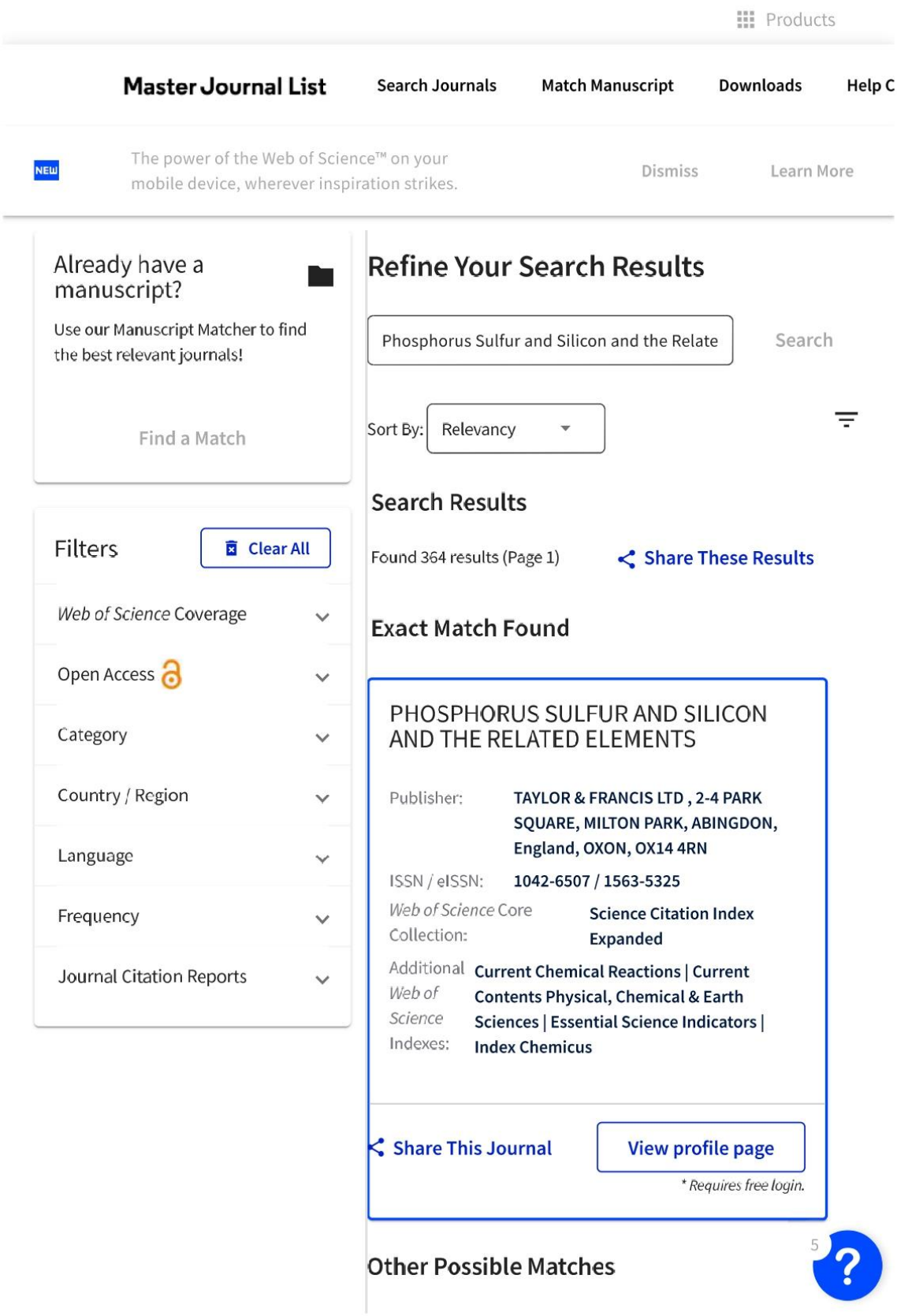
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Volume 197, 2022 - Issue 3: ICAMS-21 e-Conference; Guest Editor: Dr. Mohanraj

Articles

Chemical and sweet basil leaf mediated synthesis of cerium oxide (CeO_2) nanoparticles: Antibacterial action toward human pathogens

S. Sebastiammal, N. Annlin Bezy, A. Somaprabha, J. Henry, C.S. Biju & A. Lesly Fathima

Pages 237-243 | Received 11 Aug 2021, Accepted 07 Dec 2021, Published online: 22 Dec 2021

Cite this article https://doi.org/10.1080/10426507.2021.2017435 Check for updates

Abstract

The current study explores the bacterial inactivation of CeO_2 nanoparticles (NPs) synthesized via chemical co-precipitation (C-CeO_2) and green synthesis (G-CeO_2) route. In the green synthesis route, the sweet basil leaf extract is used as a reducing agent while CTAB acts as a surfactant in the chemical route. The structural, surface, and optical properties were studied by different physico-chemical techniques. X-ray diffraction pattern of CeO_2 nanoparticles confirms face-centered cubic (FCC) crystal system. The crystallite size is reduced for the green synthesized CeO_2 nanoparticles.

Scopus Preview

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Scopus coverage years: from 2006 to Present

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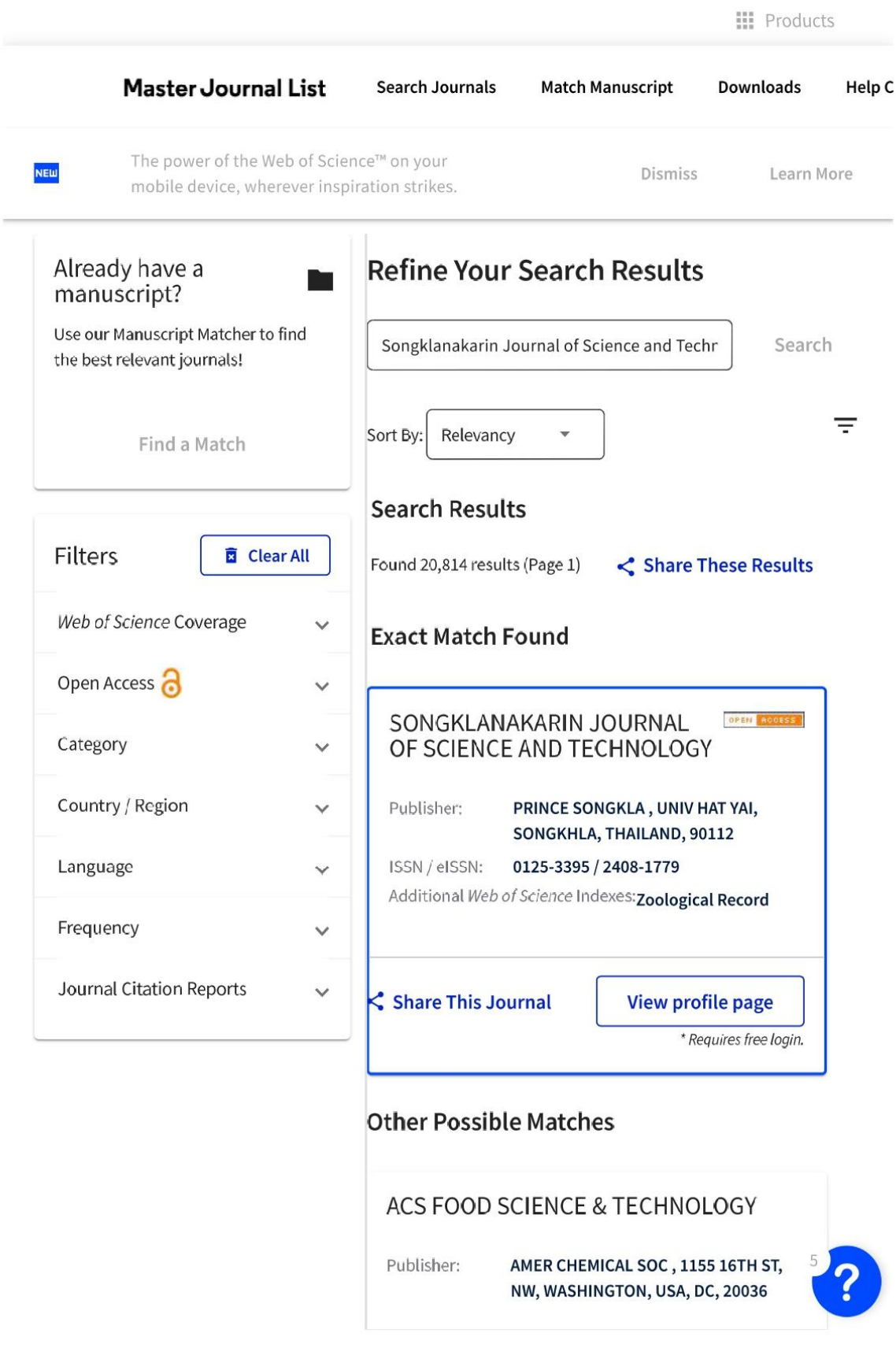
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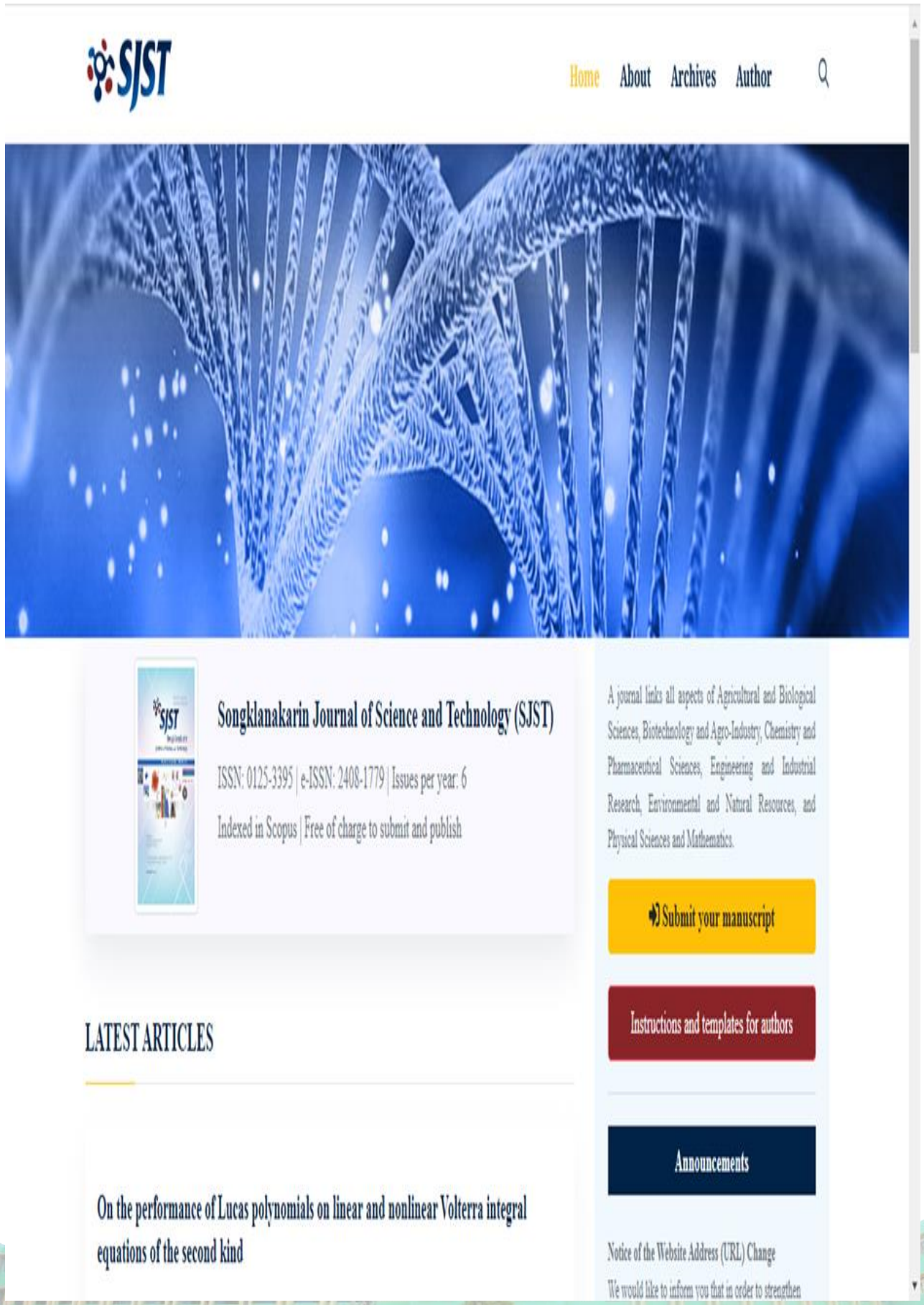
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Original Article

Green synthesis of cerium oxide nanoparticles using *aloevera leaf* extract and its optical properties

S. Sebastiammal[1], S. Sonia[1], J. Henry[2], and A. Lesly Fathima[1*]

[1] *Department of Physics, Holy Cross College (Autonomous), Nagercoil, Tamil Nadu, 629004 India*

[2] *Department of Physics, Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli, Tamil Nadu, 627012 India*

Received: 11 February 2020; Revised: 20 March 2020; Accepted: 13 April 2020

Abstract

In the present report, bio-reduction of cerium nitrate into cerium oxide nanoparticles has been done using *aloevera* leaf extract. The synthesized CeO_2 nanoparticles were characterized by PXRD, FTIR, UV-DRS, FESEM, EDAX and PL. From the PXRD analysis, it is found that the synthesized CeO_2 nanoparticles were the face centered cubic structure. The crystalline size is found to be about 7 nm and 12 nm for the CeO_2 nanoparticles before and after calcination respectively. FTIR spectra exhibit the formation of CeO_2 nanoparticles. The UV – Vis spectra shows an absorption peak at 320 nm. The FESEM analysis, showed spherical shaped CeO_2 nanoparticles and its size is about 50 nm.

Keywords: biosynthesis, CeO_2 NPs, PXRD, FTIR, UV-DRS, FESEM

1. Introduction

There is an increasing commercial demand for nanoparticles due to its promising applications in electronics, chemistry, catalysis, energy and medicine (Bar *et al.*, 2009; Mittal & Pandey, 2014). Metallic nanoparticles are traditionally synthesized by wet-chemical techniques, where the chemicals used are quit toxic and inflammable (Edison & Sethuraman, 2013). Cerium is one of the most abundant rare-earth metals found in the Earth's crust (Nisha *et al.*, 2014). Cerium oxide (CeO_2) has received much attention in the global nanotechnology market due to its useful applications for catalysts, fuel cells, and fuel additives (Bankar, Joshi, Kumar, & Zinjarde, 2010). CeO_2 is a semiconductor with wide band gap energy (3.19 eV) and large exciton binding energy (Arumugam *et al.*, 2015). Recently the CeO_2 NPs were used as a diesel fuel additive, to reduce the ignition temperature of carbonaceous diesel exhaust particle (DEP) and subsequently to reduce the emission of particulate matter from diesel engines (Niu, Azfer, Rogers, Wang, & Kolattukudy, 2007). Cerium oxide nanoparticles are exhibiting excellent antioxidant properties so that they can be able to cure stress-related diseases (Caputo *et al.*, 2017).

Green nanotechnology is a mushrooming area of research in the scientific world. The green synthesis method offers a plenty of advantages such as cost-effectiveness, large scale commercial production and pharmaceutical applications. The plant extract which facilitates green synthesis has gained a wide attention and has emerged as an active research area in the field of nanotechnology. Plant extract consists of tannins and poly phenol which are widely applied in food processing as natural additives to edible foods and in leather industry for fabrication. The polyphenolic OH^- groups have good affinity towards metal ions; hence the plant extract is widely applied as reducing, stabilizing and chelating agent (Kalaiselvi, Mathammal, Vijayakumar, & Vaseeharan, 2018). Arunachalam, Karpagasundaram, and Rajarathinam, (2017) have prepared *Prosopis juliflora* leaf extract mediated CeO_2 nanoparticles and studied its antibacterial activity

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Source details

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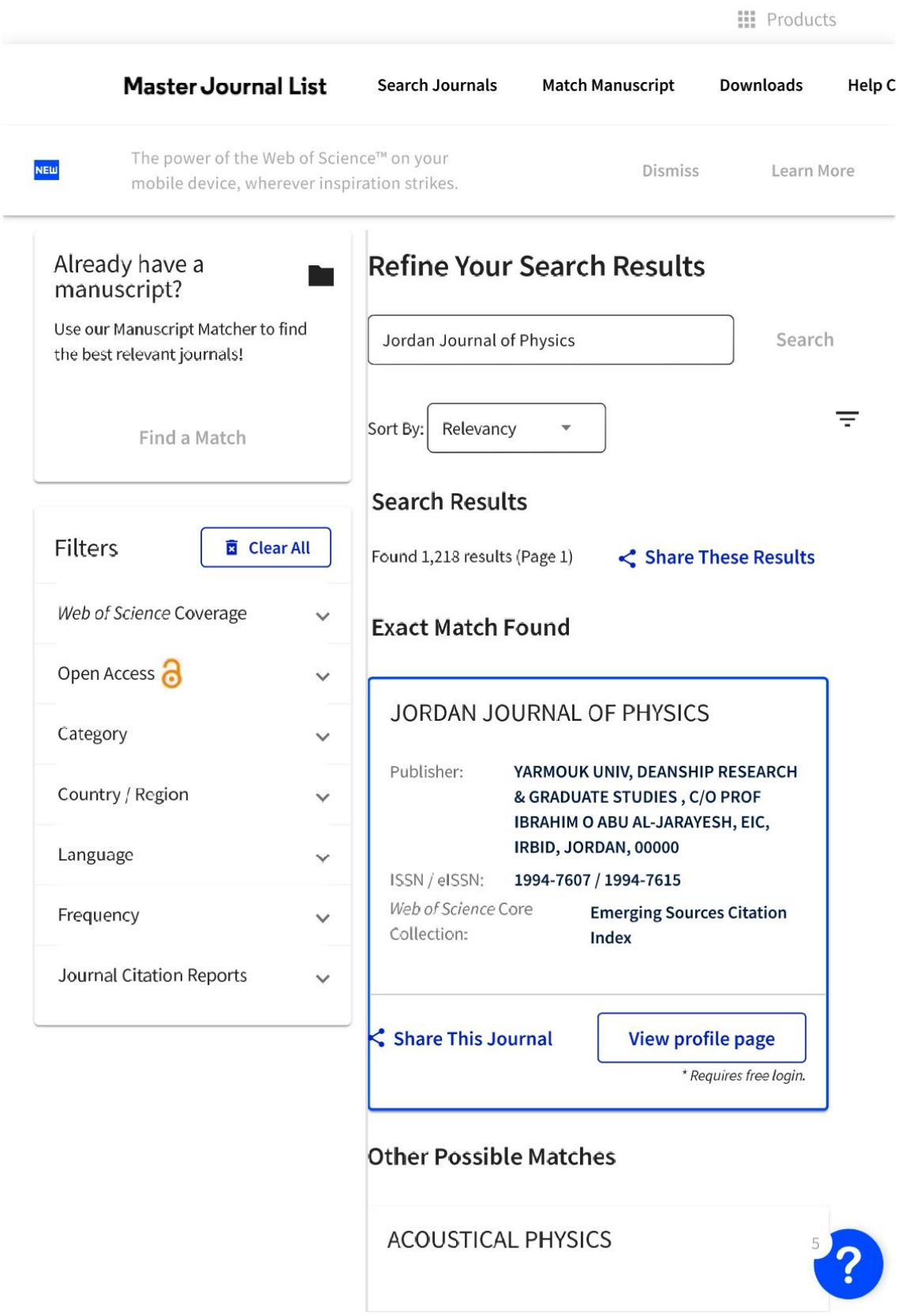
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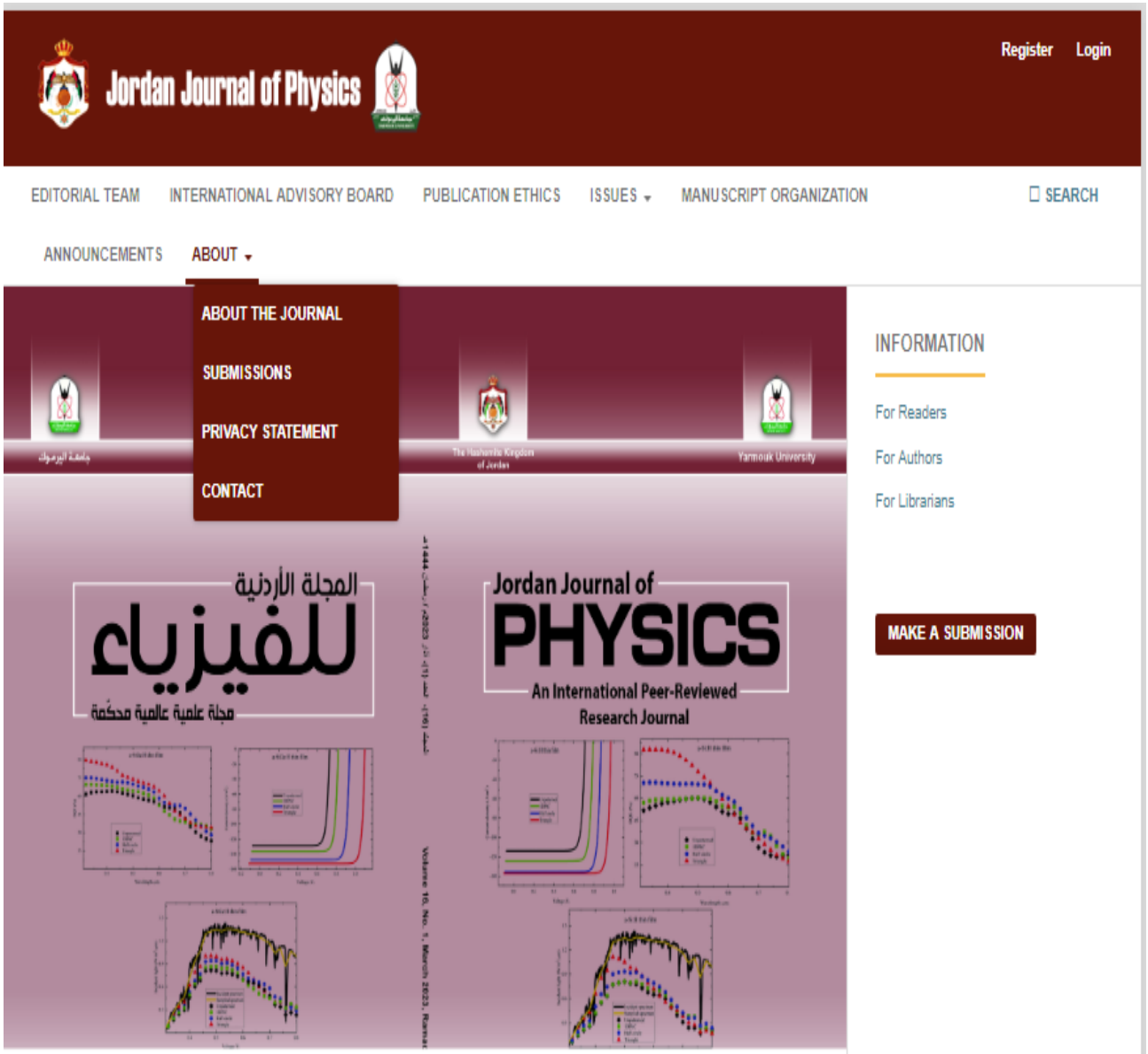
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Volume 14, Number 5, 2021. pp. 437-444

Jordan Journal of Physics

ARTICLE

Albumen-assisted Synthesis of Nanocrystalline Nickel Ferrite Photocatalyst

P. Aji Udhaya[a,b], **M. Meena**[c], **M. Abila Jeba Queen**[a], **M. Mary Freeda**[a] and **T. Regin Das**[d]

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[b] *Research Scholar, Reg. No. 18123152132038, Department of Physics, S.T. Hindu College, Nagercoil, Affiliated to Manonmaniam Sundaranar University, Abishekapatti, Tirunelvel-627012, India.*

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[d] *Department of Physics, Lekshmipuram Arts and Science College, Neyyoor, Nagercoil, India.*

Doi: **https://doi.org/10.47011/14.5.5**

Received on: 01/05/2020; *Accepted on: 15/09/2020*

Abstract: As a simple step to remove the polluting dyes in aqua ecosystem, $NiFe_2O_4$ nanoparticles well known for their ferromagnetic properties, low conductivity and high electrochemical stability were prepared by simple auto combustion method using egg white as fuel *via* green synthesis route. The structural, morphological and magnetic properties of prepared $NiFe_2O_4$ was analyzed. The desirable phase purity of the prepared spinel ferrite was deliberated by X-ray Diffractometer (XRD), Fourier Transform Infrared Spectrometer (FTIR), Scanning Electron Microscopy (SEM), Energy Dispersive and Vibrating Sample Magnetometer (VSM). XRD predicts the phase formation, particle size and lattice parameter of the spinel ferrite. The FTIR spectrum confirms the ferrite structure. The morphological and elemental analysis was made using SEM and EDAX. The hysteresis curve reveals the magnetic properties, such as remanence magnetization (Mr), coercivity (H_c) and saturation magnetization (M_s). The photocatalytic efficiency of the synthesized samples was determined from degradation of methylene blue dye. The whole process was monitored using spectrophotometer at regular intervals of time. The maximum photocatalytic degradation efficiency for $NiFe_2O_4$ is around 95.6 %.

Keywords: $NiFe_2O_4$, Ferrite, Green synthesis, Egg white, Combustion, Photocatalyst.

1. Introduction

Wastewater management in developing countries is a major problem due to various industrial processes that meet human needs. Dyeing and pigment industries are of major environmental concern among the various industries, as wastewater includes several non-biodegradable organic colors. From textiles to food, dyes are widely used by humans. Methylene blue is an organic dye that is synthetic and water soluble. It is widely used as a colorant in textiles, paper, plastics, cosmetics, leather, food and many other industries, leading to large dye effluent discharges. If the effluents are not treated properly, they become a serious environmental problem that affects the flora and fauna, as well as human health. Methylene blue dye can irradiate the eyes and skin and damage the respiratory, reproductive, and nervous systems through carcinogenic actions. In

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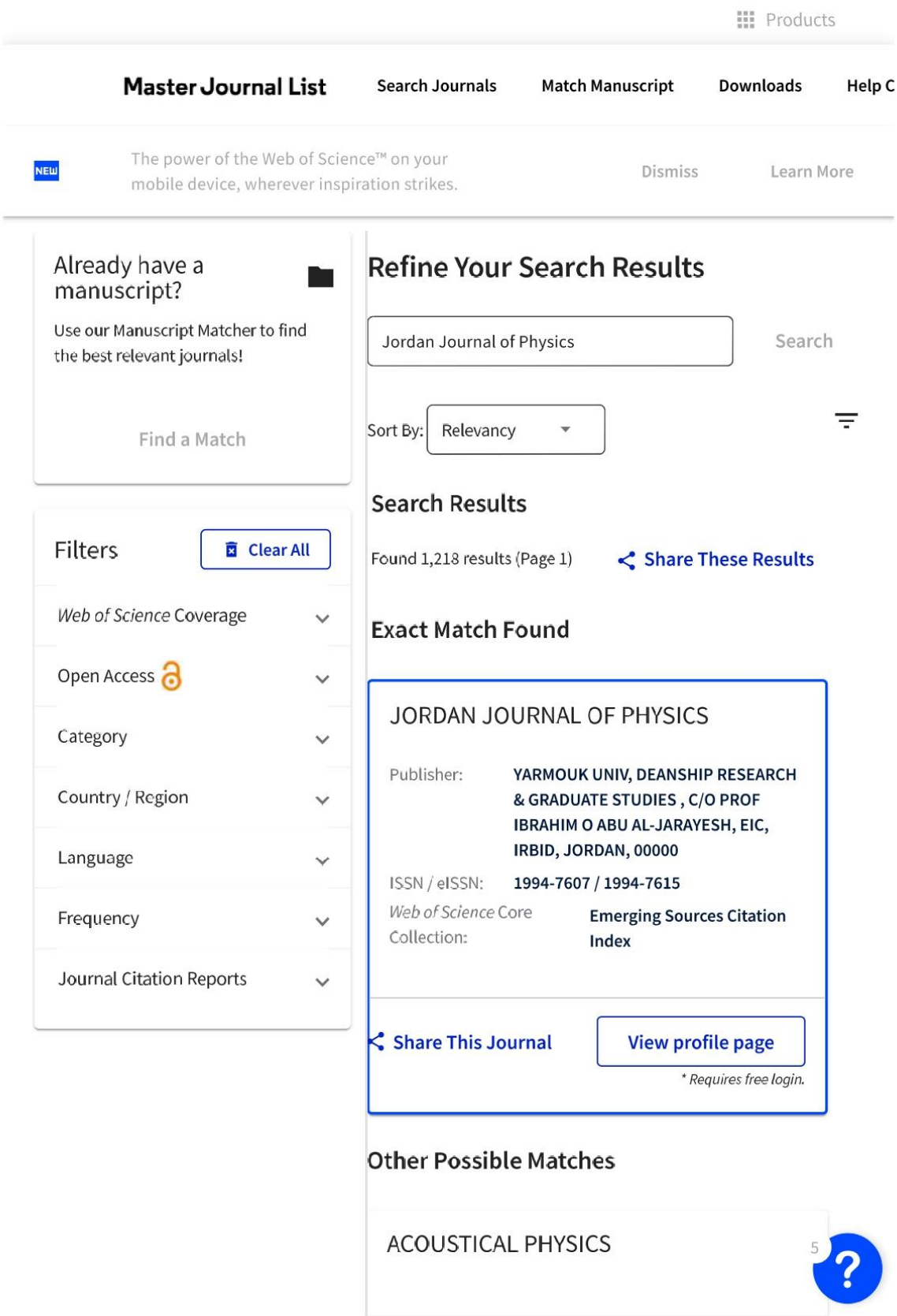
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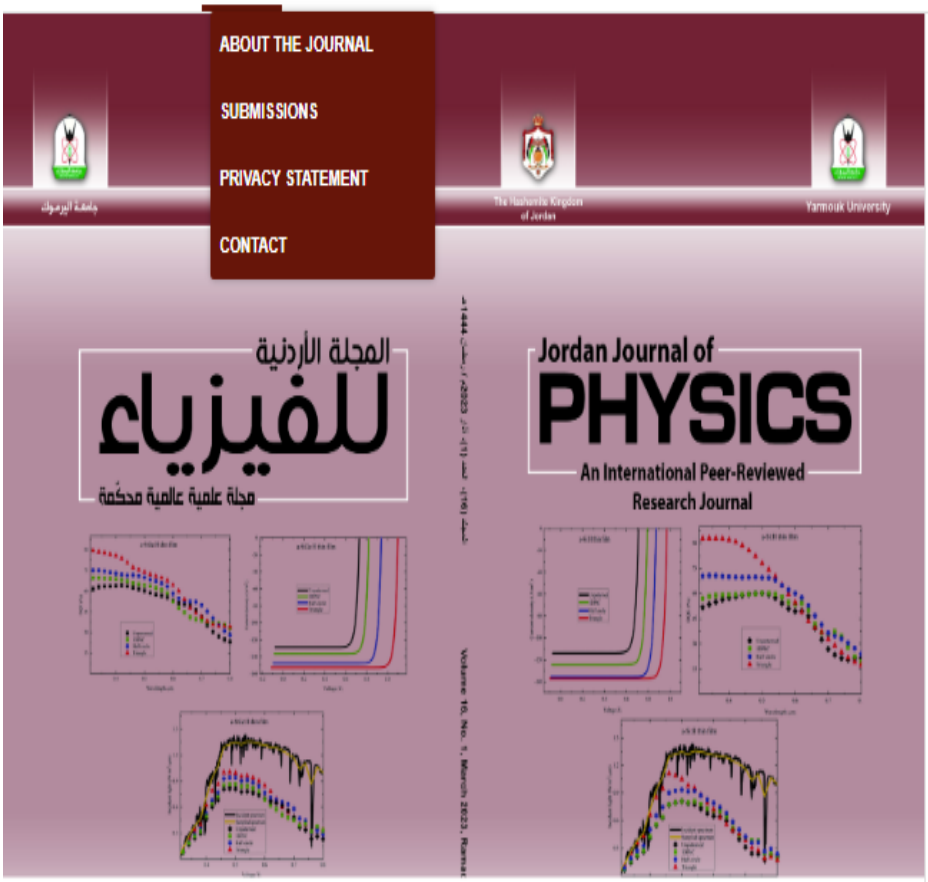

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Jordan Journal of Physics

ARTICLE

Albumen-mediated Green Synthesis of $ZnFe_2O_4$ Nanoparticles and Their Physico-Chemical Properties

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Abstract: Spinel ferrites with general formula AB_2O_4 possess charming magnetic and electrical properties owing to their thermal and chemical steadfastness. Spinel zinc ferrite ($ZnFe_2O_4$) nanoparticles have attracted massive attention due to their unusual amalgamation of properties, especially magnetic properties, where these properties are equipped as suitable candidates in the field of electronics. Here, a simple self-combustion technique is made with the assistance of albumen to synthesize nanocrystalline zinc ferrite ($ZnFe_2O_4$) particles. The egg white (albumen) that is used in the synthesis process plays the fuel role in the process of combustion. The results of the powder X-ray diffraction (PXRD) and Fourier Transform Infrared Spectroscopy (FTIR) suggested that the synthesized nanoparticles are of single phase and show spinel structure. The photoluminescence studies reported a doublet peak at around 360-380 nm. The functional groups present in the synthesized nanoparticles were revealed from FTIR data. EDX findings give an account of the percentage composition of the elements Fe, Zn and O present in the synthesized sample. High-resolution Scanning Microscope (HRSEM) reveals the agglomerated coalescence nature of ferrite nanoparticles.

Keywords: Ferrite, PXRD, FTIR, HRSEM, EDX Albumen.

1. Introduction

Ferrites are of interest due to their electrical, magnetic and mechanical properties, which can be adapted to the requirements of device manufacturing and biological applications. Magnetic Nanoparticles have emerging biomedical applications in sundry areas, such as disease diagnostics, magnetic resonance imaging, sensors, actuators, magnetic storage devices, … etc. Nano-sized ferrites of the MFe_2O_4 type are the most significant magnetic materials which have yet to be properly investigated on the way to their physical and chemical properties. The metal-iron ratio plays a crucial role in the regulation of MFe_2O_4 nanoparticles' magnetic properties [1, 2]. Due to the increased volume fraction of surface atoms, surface effects may be crucial when reducing

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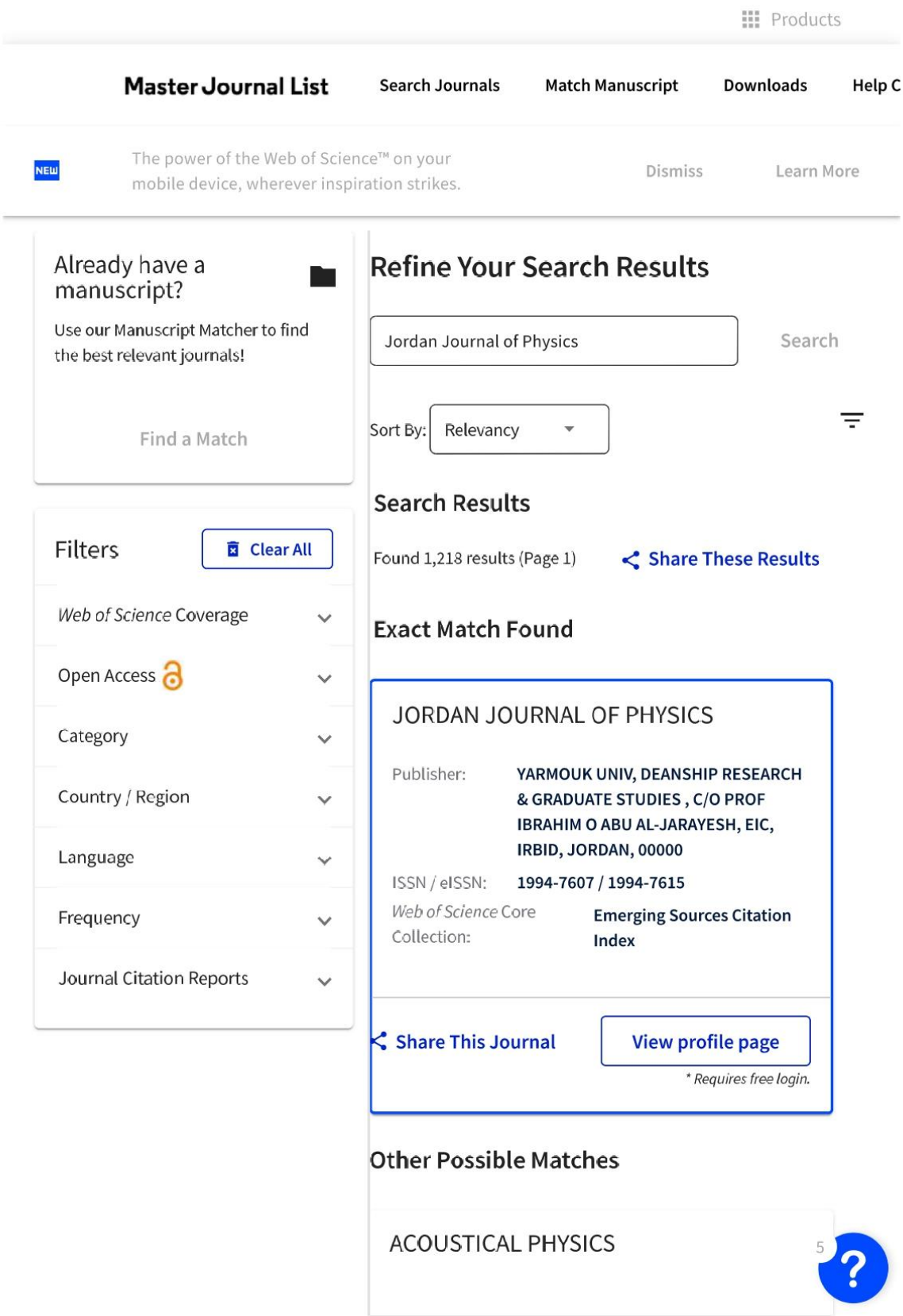
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ARTICLE

Physicochemical Properties and Antimicrobial Potential of Green Synthesized Cerium Oxide (CeO_2) Nanoparticles from Pomegranate Peel Extract

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Abstract: Green synthesis of CeO_2 Nanoparticles (NPs) with small size and high stability paved the approach to recover and protect the environment by decreasing the use of toxic chemicals and eliminating biological risks in biomedical applications. Peel-mediated synthesis of CeO_2 NPs is gaining more importance owing to its easiness and eco-friendliness. In this study, biosynthesis of CeO_2 NPs using the fruit peel extract of *punica granatum* is reported. The synthesized CeO_2 NPs are characterized by Powder X-ray Diffraction (PXRD), UV-Diffused Reflection Spectroscopy (UV-DRS), Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-Ray Analysis (EDAX) and antimicrobial activity. The CeO_2 NPs show more lethal activity towards gram +ve bacteria than towards gram –ve bacteria.

Keywords: Biosynthesis, Optical properties, Antimicrobial activity.

Introduction

Pathogenic microorganisms have become a major problem in our today life, since they pose a threat to health and food materials. This paves the way to the research community to investigate solutions to remove or reduce these hazardous species from the environment. Emergence of new bacterial strains which are resistant to current antibiotics has become a serious health issue. From recent literature, it is believed that nanotechnology is one of the most active research areas in providing solutions for such problems. Synthesis of nanoparticles (NPs) with various sizes and shapes has gained much importance in nanotechnological applications [1-5]. In general, nanoparticles have a higher surface-to-volume ratio with an enlarged contact area with microbes. This feature enhances the biological activity of NPs and finds applications in the medical field.

CeO_2 is a semiconductor material which has a wide bandgap ranging between 3.0 eV and 3.9 eV with large excitation energy [6]. CeO_2 NPs have received much attention in nanotechnology due to their useful applications as catalysts, fuel cells and antioxidants in biological systems [7-10]. CeO_2 can be prepared by several methods,

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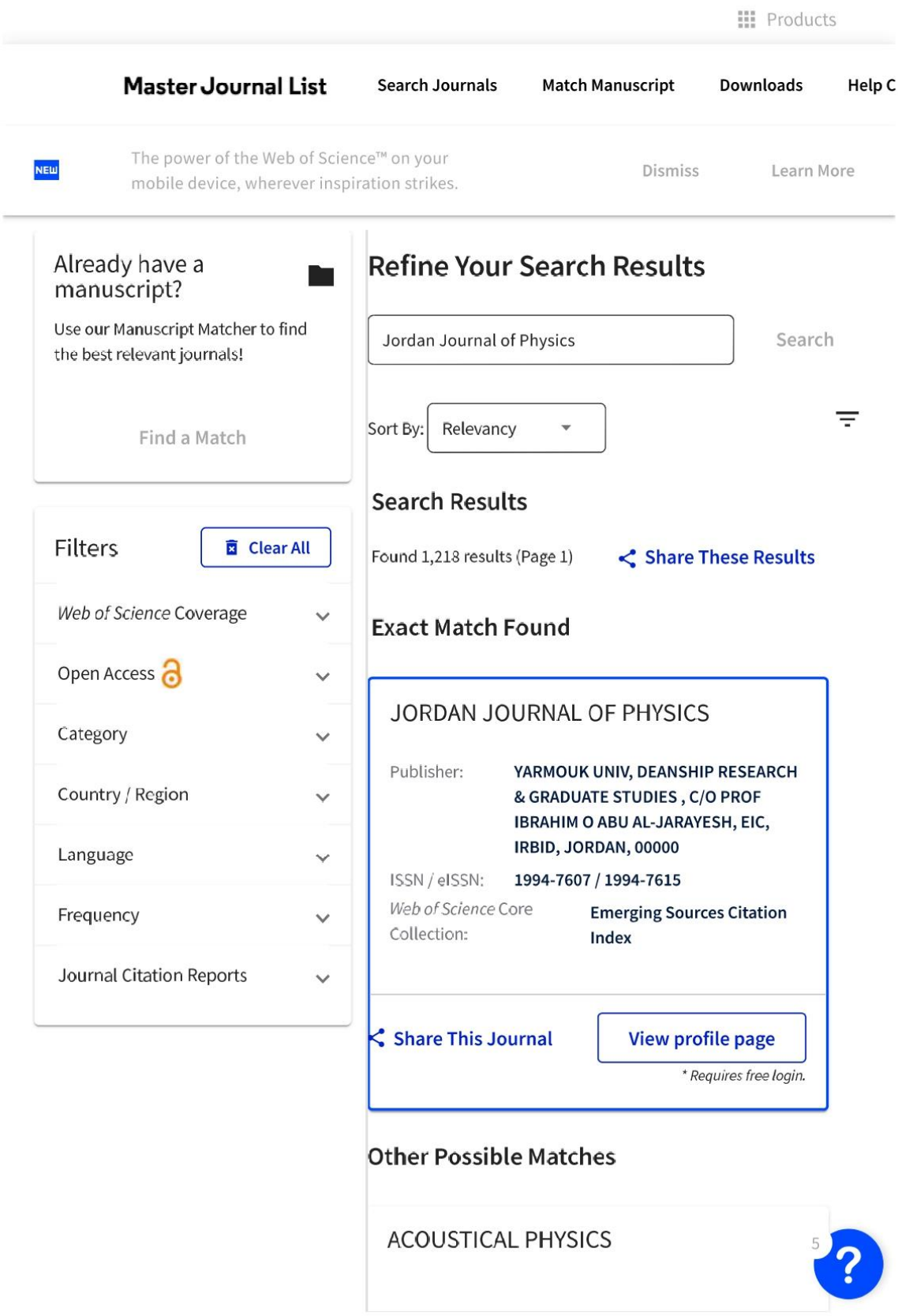
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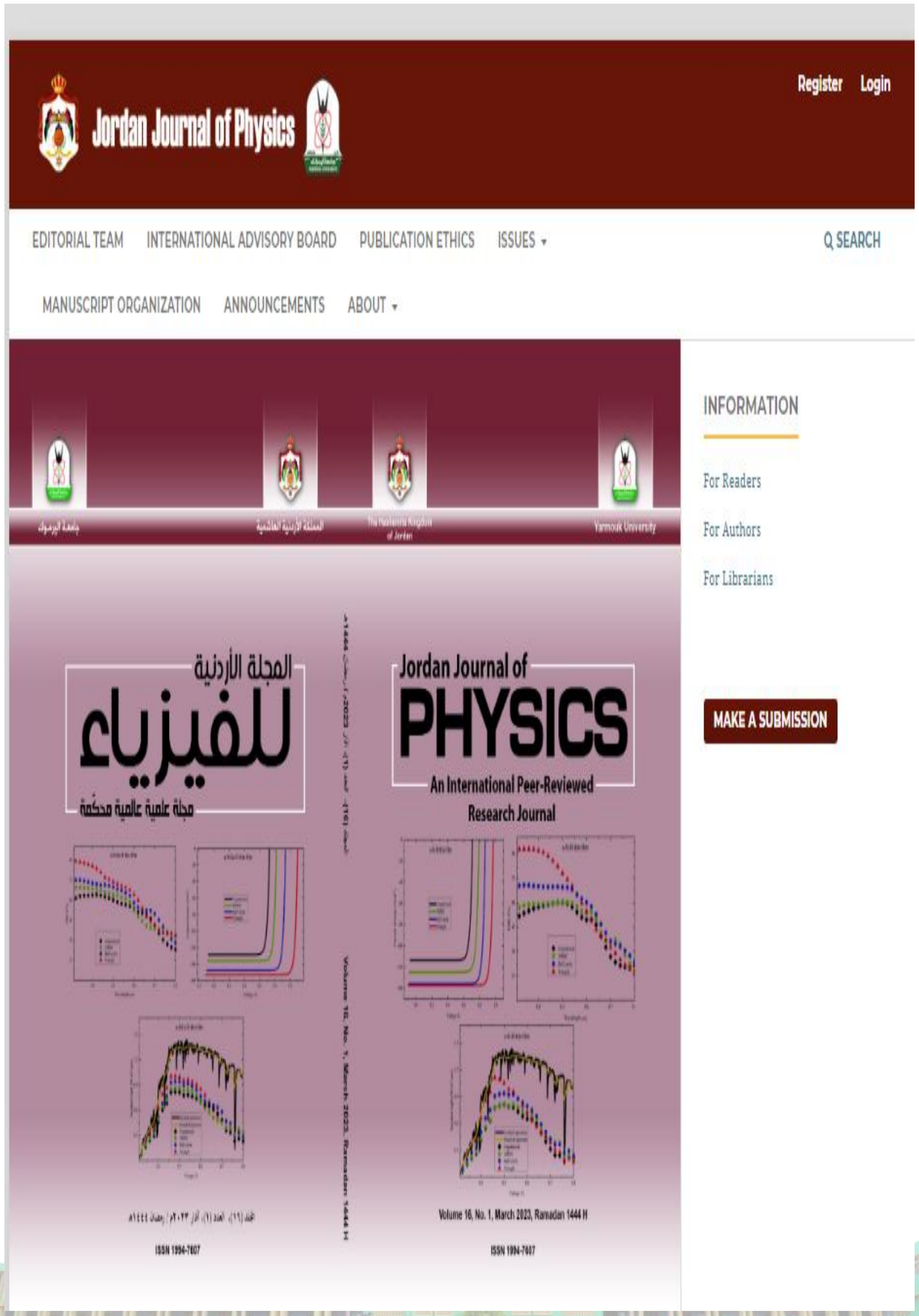
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Jordan Journal of Physics

ARTICLE

Effect of ZrO_2 Nanofiller on the Physical Properties of Epoxy Composites: Mechanical, Thermal and Dielectric

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Abstract: In this present work, Zirconia nanoparticles were prepared by precipitation method, Zirconium Oxychloride ($ZrOCl_2.8H_2O$) and ammonia (NH_3) as starting materials. The synthesized Zirconia nanoparticles were characterized by XRD and the grain size in nanoscale was confirmed. The sheets of neat epoxy resin and epoxy with addition of ZrO_2 nanoparticles are primed by solution casting method. The structures of epoxy polymer and hardener were found out using FTIR analysis. The thermal properties were analyzed using Thermo Gravimetric Analysis (TGA) and Differential Thermal Analysis (DTA). Thermo gravimetric analysis has been employed to investigate the thermal characteristics and their mode of thermal degradation. Differential thermal analysis has been used to determine the glass transition temperature of epoxy nanocomposites. The mechanical properties like tensile and flexural studies were analyzed and thus influences of nanofiller loading on these parameters were found to be very low.

Keywords: Epoxy, ZrO_2 nanoparticles, Nanocomposites, Thermal stability, Dielectric properties, Tensile strength, Flexural strength.

Introduction

Polymer nanocomposites have attracted increasing attention in the last decade because of their significant improvement of physical and chemical properties over the matrix polymers. The effects of nanofillers on these properties have been extensively observed to make nanocomposites for application purpose. The addition of just a few percent by weight of nanofillers can result in significant enhancement in dielectric, thermal and mechanical properties. The incorporation of metal oxide nanoparticles with polymer is approached to improve the mechanical strength [1–6]. The effects of inorganic fillers on the properties of composites strongly depend on filler size and shape, type of particles and the degree of dispersion [7-8]. Various nanoscale fillers, including metal oxides, montmorillonite and calcium carbonate, have been reported to enhance the mechanical properties, thermal stability, gas barrier properties, electrical properties and flame retardancy of the polymer matrix [9-11]. Among various metal oxide fillers, nano-sized zinc oxide (ZnO), zirconium oxide (ZrO_2), titanium dioxide (TiO_2) and cerium oxide (CeO_2) fillers have attracted considerable attention because of their unique physical properties as well as their low cost and extensive applications in diverse areas [12-15]. Here, the purpose of study is to evaluate the physical properties of epoxy resin with Zirconia nanoparticles.

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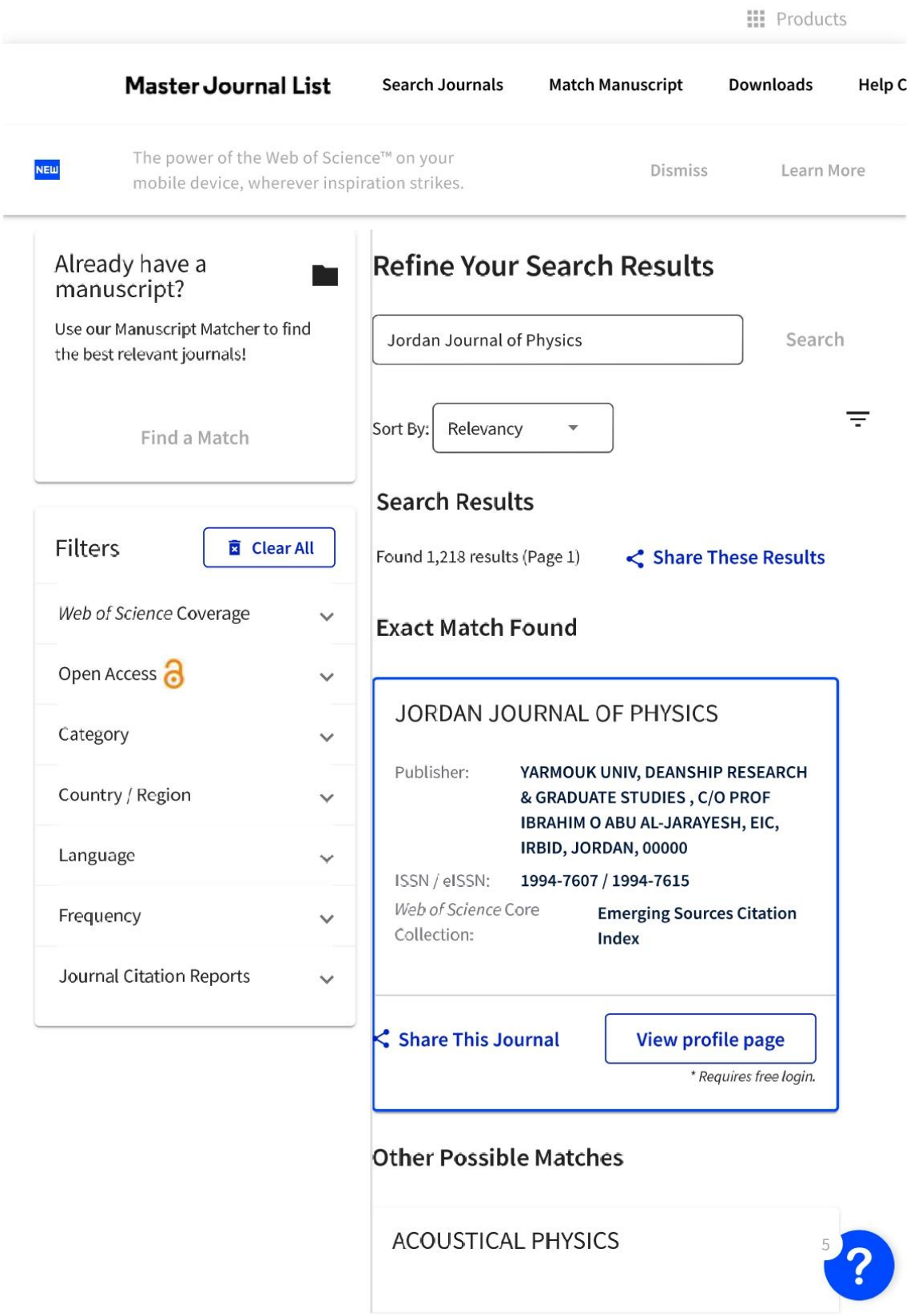
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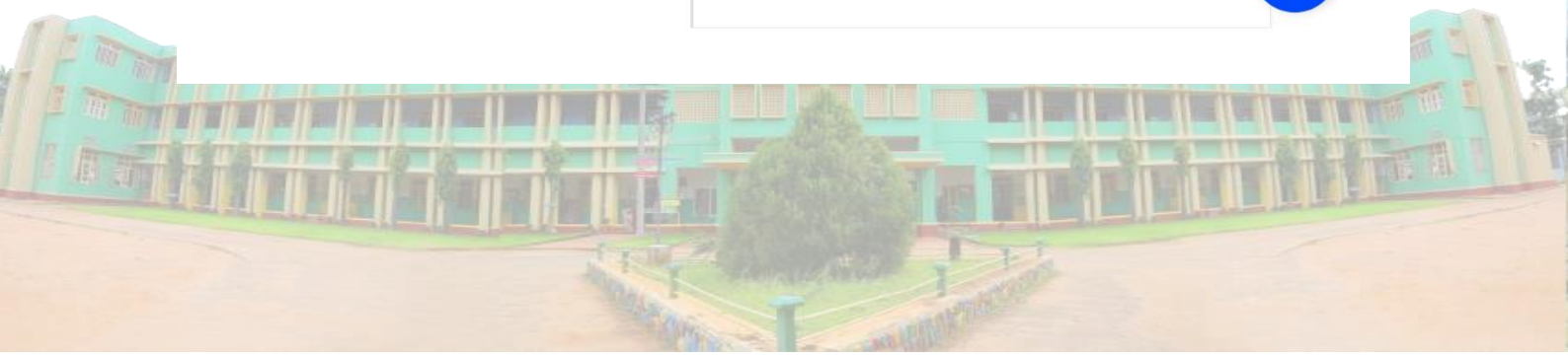

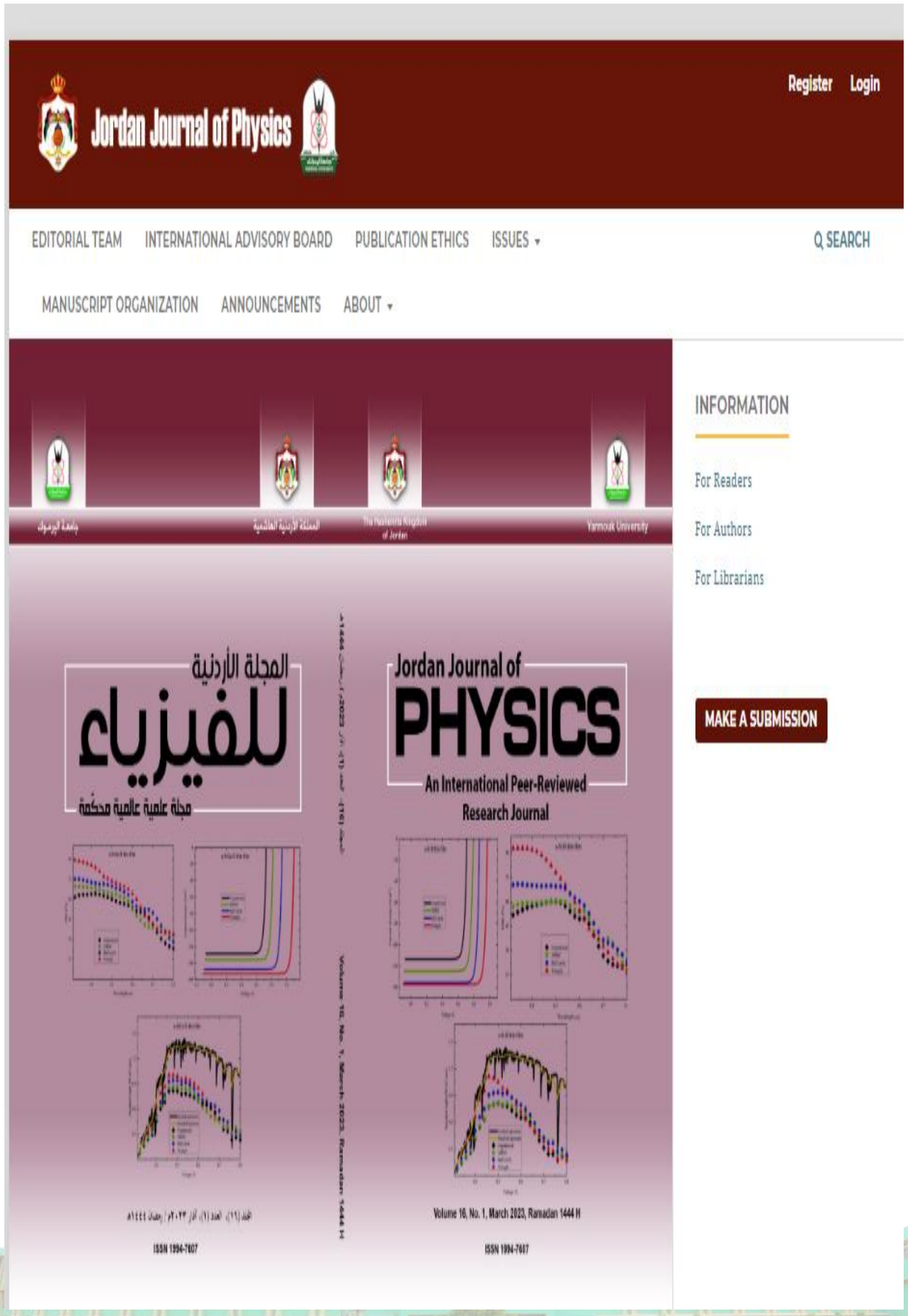
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ARTICLE

Structural and Optical Properties of Pure NiO Nanoparticles and NiO-Mn_2O_3, NiO-CdO, NiO-Pb_2O_3, NiO-ZnO Nanocomposites

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Abstract: Pure nickel oxide (NiO) nanoparticles and NiO-Mn_2O_3, NiO-CdO, NiO-Pb_2O_3, NiO –ZnO nanocomposites were synthesized by co-precipitation method. The PXRD studies revealed that NiO, Mn_2O_3 and CdO possessed cubic structure, Pb_2O_3 possessed monoclinic structure, ZnO possessed hexagonal structure and confirmed the presence of polycrystallinity nature of NiO and Mn_2O_3, CdO, Pb_2O_3, ZnO in the nanocomposites. The average grain size of NiO nanoparticles was found to be 30.10 nm using Debye Scherer's formula. The FESEM images of NiO nanoparticles and their nanocomposites revealed spherical shaped structure and NiO-Pb_2O_3 revealed needle shaped rod-like structure. EDAX analysis confirmed the composition of NiO nanoparticles and their nanocomposites. Raman spectra exhibited characteristic peaks of pure NiO and that of NiO- Mn_2O_3, NiO-CdO, NiO- Pb_2O_3, NiO-ZnO in the synthesized nanocomposites. In the PL spectra, blue and green emission was observed in the samples. UV-vis spectra revealed the absorption peaks of NiO nanoparticles and their nanocomposites. Thus, the synthesized NiO- Mn_2O_3, NiO-CdO, NiO - Pb_2O_3 and NiO-ZnO nanocomposites can be a suitable material for electrocatalysis applications.

Keywords: Nickel oxide nanocomposites, Structure, Morphology, Absorption, Luminescence.

1. Introduction

Nickel oxide (NiO) is an important transition metal oxide that has been under the extensive investigation for decades due to its interesting electronic structures, strongly affected by Ni-3d electrons [1] which are localized in space, but spread out over a wide energy range because of strong Coulomb repulsion between them [2]. The high specific surface area of NiO nanoparticles has significant implications with respect to the energy storage devices based on electrochemically active sites (batteries, super capacitors) and energy conversion devices depending on catalytic sites or defect structures. NiO nanoparticles and their nanocomposites have been synthesized *via* a cost-effective and highly convenient co-precipitation method [3]. Mn_2O_3 nanoparticles can be utilized for advanced materials in batteries, as well as other applications, such as water treatment and imaging contrast agents [4]. CdO has potential applications in flat panel displays, organic light emitting diodes, optoelectronic devices, gas sensors and electrodes [5]. CdO also possesses both antibacterial and anticancer activity. Previous studies reported the synthesis of nanocomposites containing CdO and other metal oxide combinations [6]. The Pb_2O_3 nanoparticles are used in magnetic resonance and as magnetic nanoparticles for magnetic data storage and magnetic resonance imaging (MRI). The most

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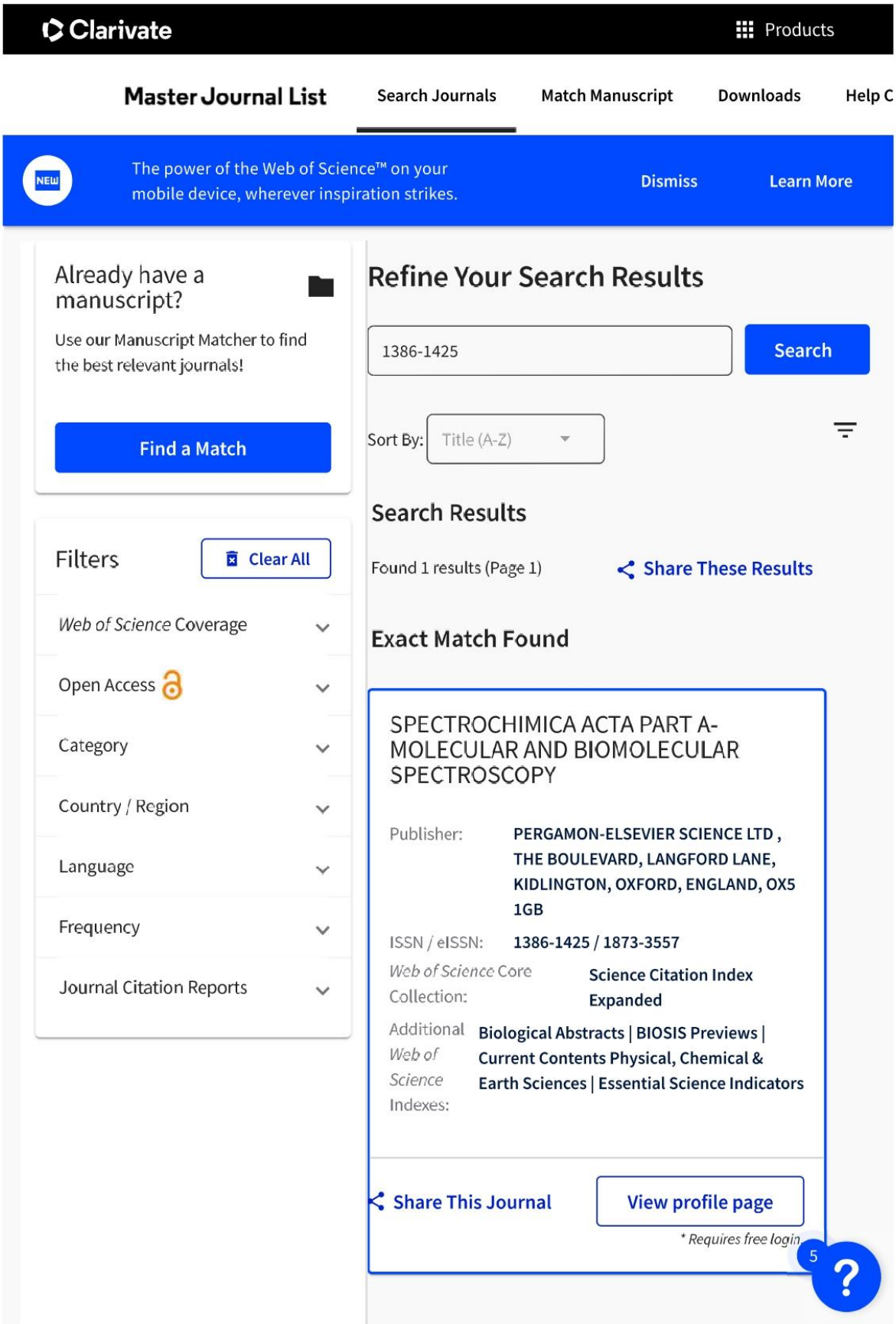
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Quantum chemical insight into molecular structure, NBO analysis of the hydrogen-bonded interactions, spectroscopic (FT–IR, FT–Raman), drug likeness and molecular docking of the novel anti COVID-19 molecule 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluorophenyl)acetamide - dimer

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ABSTRACT

Novel antiviral active molecule 2- [(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluoro- phenyl)acetamide has been synthesised and characterized by FT-IR and FT-Raman spectra. The equilibrium geometry, natural bond orbital calculations and vibrational assignments have been carried out using density functional B3LYP method with the 6-311G++(d,p) basis set. The complete vibrational assignments for all the vibrational modes have been supported by normal coordinate analysis, force constants and potential energy distributions. A detailed analysis of the intermolecular interactions has been performed based on the Hirshfeld surfaces. Drug likeness has been carried out based on Lipinski's rule and the absorption, distribution, metabolism, excretion and toxicity of the title molecule has been calculated. Antiviral potency of 2- [(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluoro-phenyl) acetamide has been investigated by docking against SARS-CoV-2 protein. The optimized geometry shows near-planarity between the phenyl ring and the pyrimidine ring. Differences in the geometries due to the substitution of the most electronegative fluorine atom and intermolecular contacts due to amino pyrimidine were analyzed. NBO analysis reveals the formation of two strong stable hydrogen bonded N–H···N intermolecular interactions and weak intramolecular interactions C–H···O and N–H···O. The Hirshfeld surfaces and consequently the 2D-fingerprint confirm the nature of intermolecular interactions and their quantitative contributions towards the crystal packing. The red shift in N–H stretching frequency exposed from IR substantiate the formation of N–H···N intermolecular hydrogen bond. Drug likeness and absorption, distribution, metabolism, excretion and toxicity properties analysis gives an idea about the pharmacokinetic properties of the title molecule. The binding energy −8.7 kcal/mol of the nonbonding interaction present a clear view that 2- [(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluoro- phenyl) acetamide can irreversibly interact with SARS-CoV-2 protease.

1. Introduction

Pyrimidine and its derivatives take up a key position in the field of medicinal chemistry due to its multifarious pharmacological activities. In an urge for searching new promising small therapeutic agents, we introduce 2- [(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluoro- phenyl) acetamide (DAPF). In the present study, we focus on the investigation on the molecular structure, electronic properties, vibrational spectra and molecular docking of the title compound, with the hope that the results of the present investigation may be decisive in the prognosis of its mechanism of biological activity.

Pyrimidines, the fundamental building blocks for nucleic acids, are invoking much scientific interest owing to their potential biological activities and pharmacological applications [1]. Pyrimidines are also reported to show anti-HIV, [2] antidengue [3] and anticancer [4] activities. The title compound DAPF, which has the amino substituent at the 4,6- position are found to be Troponin I-Interacting Kinase

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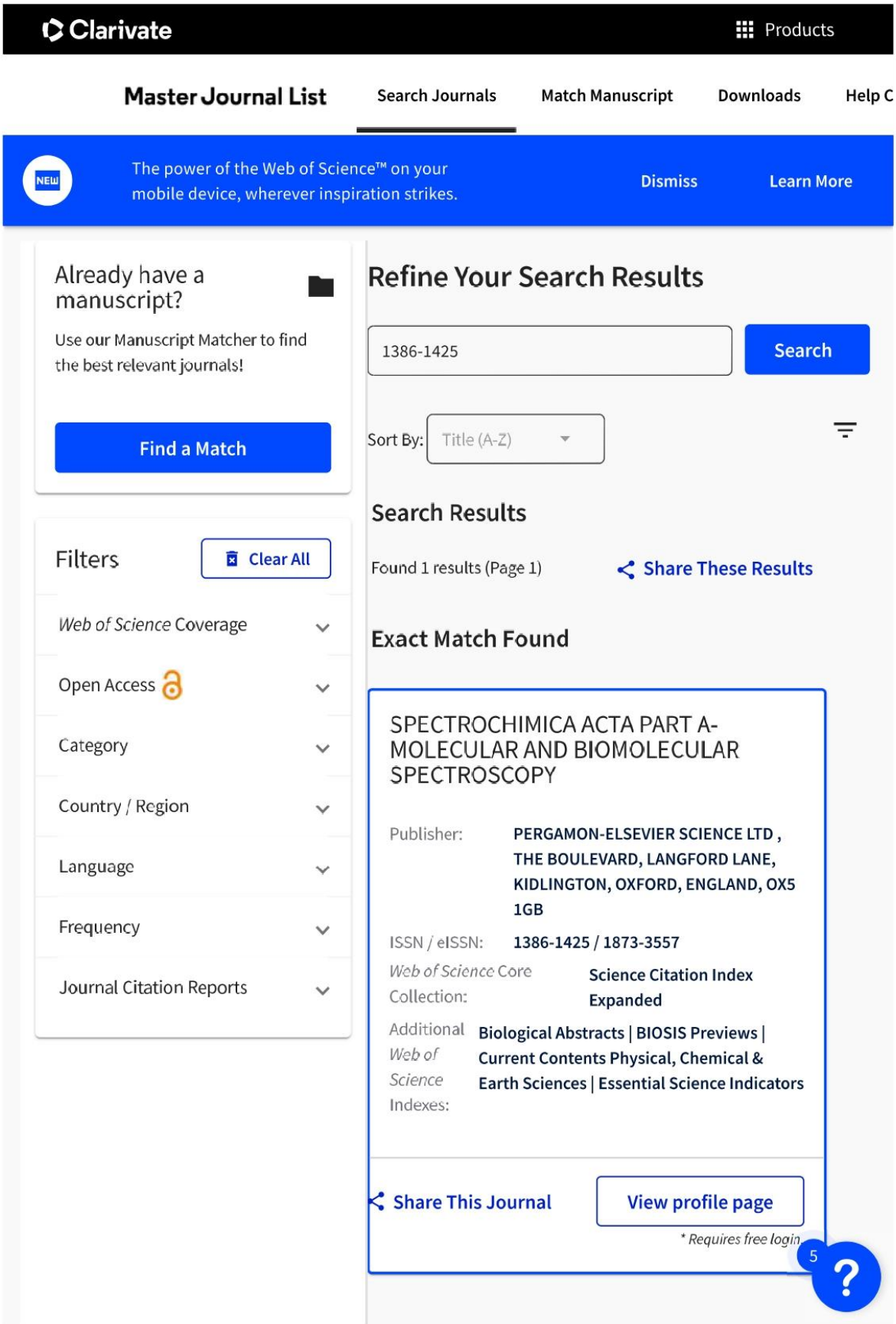
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Molecular structure, NBO analysis of the hydrogen-bonded interactions, spectroscopic (FT–IR, FT–Raman), drug likeness and molecular docking of the novel anti COVID-2 molecule (2E)-N-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]-hydrazinecarbothioamide (Dimer) - quantum chemical approach

S.J. Jenepha Mary [a,1], Sayantan Pradhan [b], C. James [a,*]

[a] Department of Physics and Research Centre, Scott Christian College (Autonomous), Nagercoil 629003, Tamil Nadu, Affiliated to Manonmaniam Sundarnar University, Abishekapatti, Tirunelveli 627012, India
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HIGHLIGHTS

- N—H···O intermolecular interactions elucidates the effect of hyperconjugation.
- C—H···O intermolecular interactions elucidates the effect of rehybridization.
- FT-IR and FT-Raman spectral analysis substantiates the red shift and blue shift in stretching frequencies.
- Drug likeness and ADMET analysis reveals pharmacokinetic properties.
- Molecular docking shows the interaction of MCMH with SARS-CoV-2 protease.

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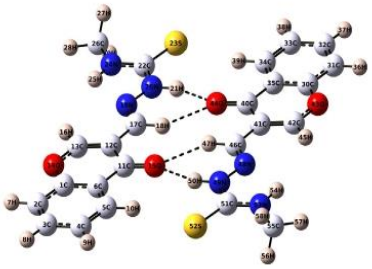

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(2E)-N-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]-hydrazinecarbothioamide

ABSTRACT

Prospective antiviral molecule (2E)-N-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]-hydrazinecarbothioamide has been probed using Fourier transform infrared (FTIR), FT-Raman and quantum chemical computations. The geometry equilibrium and natural bond orbital analysis have been carried out with density functional theory employing Becke, 3-parameter, Lee-Yang-Parr method with the 6-311G++(d, p) basis set. The vibrational assignments pertaining to different modes of vibrations have been augmented by normal coordinate analysis, force constant and potential energy distributions. Drug likeness and oral activity have been carried out based on Lipinski's rule of five. The inhibiting potency of 2(2E)-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]-hydrazinecarbothioamide has been investigated by docking simulation against SARS-CoV-2 protein.

The optimized geometry shows a planar structure between the chromone and the side chain. Differences in the geometries due to the substitution of the electronegative atom and intermolecular contacts due to the chromone and hydrazinecarbothioamide were analyzed. NBO analysis confirms the presence of two strong stable hydrogen bonded N—H···O intermolecular interactions and two weak hydrogen bonded C—H···O interactions. The red shift in N—H stretching frequency exposed from IR substantiates the formation of N—H···O intermolecular hydrogen bond and the blue shift in C—H stretching frequency

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^{1}H NMR – A validation tool for supramolecular complexes of α-cyclodextrin with Antidiabetic drugs

S. Lizy Roselet [a], J. Prema Kumari [b]

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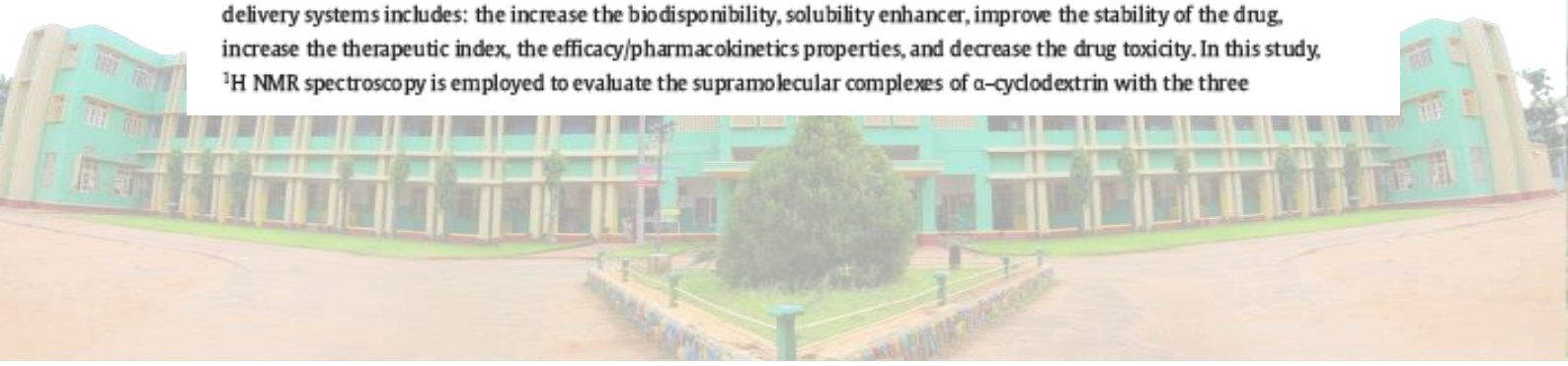
Abstract

Metformin hydrochloride, Pioglitazone hydrochloride and Glimepiride are antidiabetic drugs used in the treatment of Type–2 diabetes. In this study, supramolecular complexes of these three drugs were synthesized and characterized using ^{1}H NMR spectroscopy. The possible encapsulation of the drugs inside the supramolecular complexes were depicted according to the chemical shift variances of ^{1}H NMR of the host and guest molecules inside the inclusion complex. Nuclear Magnetic Resonance spectroscopy has been extensively employed in Chemistry and can be considered as one of the most complete spectroscopic techniques, due to its widefield of applications from structural elucidation of structures to investigations on intra/inter-molecular. ^{1}H NMR spectroscopy served as a validation tool for the supramolecular complexes. Therefore the supramolecular complexes could be used in enhancing the physico-chemical properties of the drugs thereby improving the efficacy of the drugs in the pharmaceutical industry.

Introduction

Metformin hydrochloride, Pioglitazone hydrochloride and Glimepiride are antidiabetic drugs used in the treatment of Type–2 diabetes. Cyclodextrins(CDs) are cyclic oligomers of glucopyranose units that play an important role as a host in inclusion complexes, where non–covalent interactions are involved. They have been extensively studied in supramolecular chemistry. Because of its biocompatibility, relatively non–toxicity and relatively low price, CDs have been widely employed for encapsulation of several substances, being used in food, cosmetic and pharmaceutical industries. Nuclear Magnetic Resonance spectroscopy has been extensively employed in Chemistry and can be considered as one of the most complete spectroscopic techniques, due to its widefield of applications from structural elucidation of structures to investigations on intra/inter-molecular [1], [2], [3].

Applications of NMR on CDs chemistry is so important that no other spectroscopic technique can provide the same wealth of chemical information on the supramolecular systems and it is the only technique that provides information on the right orientation of the guest molecule inside the cavity and also on other important parameters related to the physico-chemical characteristics of the inclusion complexes [4], [5], [6], [7].The main advantages of using CDs in drug delivery systems includes: the increase the biodisponibility, solubility enhancer, improve the stability of the drug, increase the therapeutic index, the efficacy/pharmacokinetics properties, and decrease the drug toxicity. In this study, ^{1}H NMR spectroscopy is employed to evaluate the supramolecular complexes of α–cyclodextrin with the three



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Design Engineering

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Plant mediated Synthesis and Characterization of Silver Nanoparticles Using the ethanolic extract of Mangifera indica Seed and their Antimicrobial Activity

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[2]Research Department of Physics, Holy Cross College (Autonomous), Nagercoil-629004, Tamil Nadu, India.
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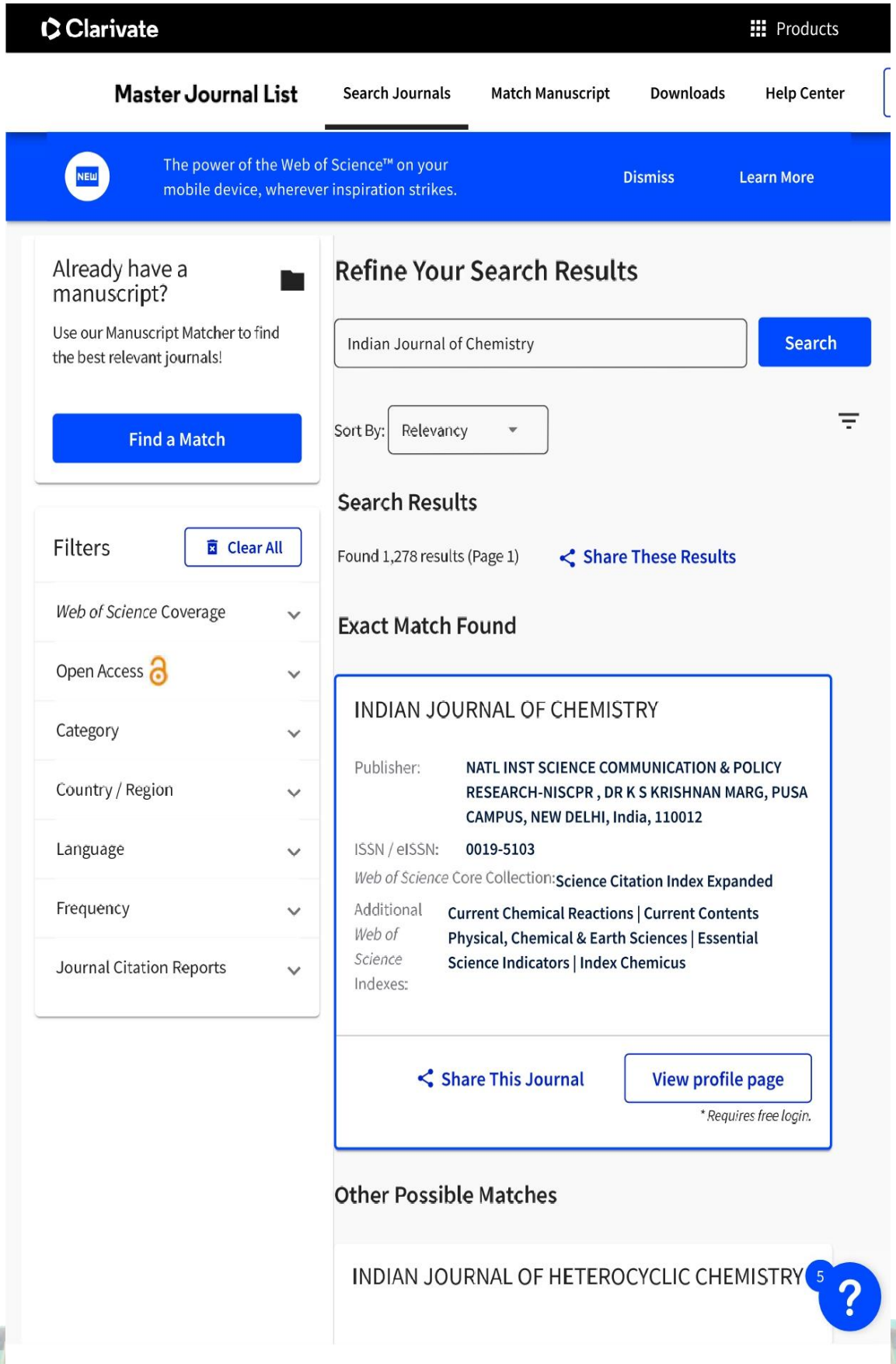
Abstract

Environment-friendly methods for the synthesis of silver nanoparticles become a valuable method in the current scenario. The utilization of phytochemicals from plant extract has become a unique skill for the synthesis of nanoparticles as they possess the dual nature of reducing and capping agents to the nanoparticles. In the present study silver nanoparticles were synthesized by using the ethanolic extract of Mangifera indica seed as a reducing and capping agent at room temperature. The formed nanoparticles were characterized by UV-Vis, FT-IR, XRD, SEM and EDAX and TEM. XRD shows the nanoparticles are crystalline. TEM shows particles are spherical and the size of the nanoparticles are in the range of 14.06 nm – 49.043 nm. FT-IR analysis shows that Mangifera indica seed extract capping in silver nanoparticles and has profound anti-microbial activity against the pathogens Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Candida albicans and Aspergillus niger.

Keywords: Silver nanoparticles, Mangifera indica, Anti-microbial activity.

1. Introduction

Nanotechnology is a significant field that deals with particles size approximately 1 to 100 nm. The chemical, physical and biological properties are differing from their bulk and their properties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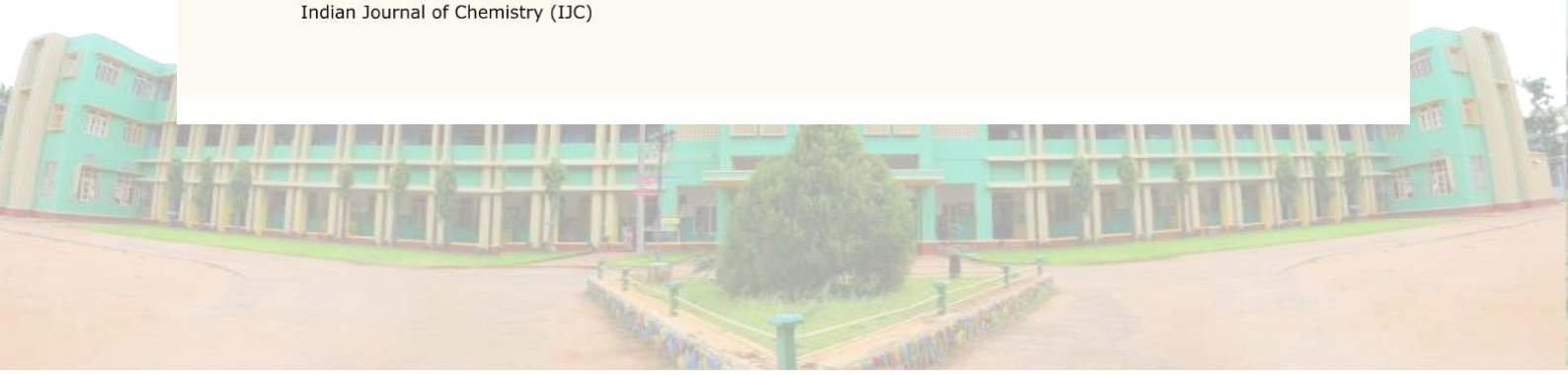

Indian Journal of Chemistry
Vol. 60B, February 2021, pp. 273-276

Computational calculations and molecular docking studies on 2-(2-ethylaminothiazol-5-oyl)benzothiazole

N S Femila Nirmal[a], Bojaxa A Rosy[b] & T F Abbs Fen Reji*[a]

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Received 16 December 2019; accepted (revised) 11 January 2021

2-(2-Ethylaminothiazol-5-oyl)benzothiazole has been synthesized and its bond length, bond angle, dihedral angle, HOMO-LUMO and Mulliken charges on the atoms have been calculated by density functional theory (DFT/B3LYP) method with 6-311++G(d,p) basis sets. Biological properties like the target receptor identification and identification of interacting residues, of this compound is identified and analyzed by using Openbabel GUI (C) software.

Keywords: DFT method, marine alkaloids, benzothiazole and molecular docking

Alkaloids have attracted the attention of humans due to their significant bioactivity. The chemical compounds, which are isolated from marine sources usually consists of nitrogen containing heterocyclic rings. Due to these promising biological activities, there has been a rapid growth of interest in the synthesis of this class of compounds and their analogues. Benzothiazole is a privileged heterocyclic scaffold found in a number of biologically important molecules and chemotherapeutic agents, which includes clinically used drugs. Based on this conjecture, we have conceived a tentative, retro synthetic analysis for the synthesis of benzothiazole analogs of alkaloid topsentin[1]. However, so far, no work has been reported on the vibrational analysis and molecular docking of 2-(2-ethylaminothiazol-5-oyl)benzothiazole (Figure 1). Hence, in the present work, a detailed vibrational analysis is carried out and for a proper understanding of the IR spectra a reliableassignment of all vibrational bands is essential. DFT calculations, particularly those based on hybrid functional methodshave evolved to a powerful quantum chemical tool for the determination of the electronic structure of molecules[2-8]. In this framework, the B3LYP hybrid exchange–correlation functional is one of the most used since it proved its ability in reproducing various molecular properties, including vibrational spectra[9-15] (Figure 2). The combined use of B3LYP functional and standard split valence basis set 6-31G(d) has been previously shownto provide an excellent compromise between accuracy and computational efficiency of vibrational spectra for large and medium-size molecules. In addition, molecular docking studies were carried out and, the mechanism of action of this compound on pancreas cancer cell line (PDB ID: BCL2), HIV-1 reverse transcriptase (PDB ID: 1RT2) and cytochrome P450 enzyme 14-alpha-demethylase of *M. tuberculosis* (PDB ID: 1EA1) is found and it is very much useful to develop efficient drugs.

Experimental Section

The title compound was prepared from 1-alkyl-3-(N,N-dimethylimidoyl)thiourea and 2-(2-bromo-acetyl)benzothiazole, which was prepared from 2-(1-hydroxyethyl)benzothiazole in DMF. The reaction mixture was stirred well and triethylamine was added. The reaction mixture was warmed at 80-85°C for 5 minutes. It was then cooled and poured into ice cold water with constant stirring. An orange precipitate thus obtained was filtered, washed with water and dried. The crude product was crystallized from methanol: water (2:1) and then from benzene:

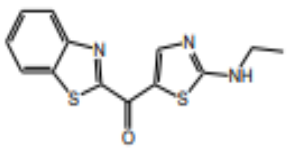

Figure 1 — Structure of 2-(2-ethylaminothiazol-5-oyl) benzothiazole

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Source details

Turkish Journal of Physiotherapy and Rehabilitation

Scopus coverage years: from 2018 to 2023

Publisher: Turkish Physiotherapy Association

ISSN: 2651-4451 E-ISSN: 2651-446X

Subject area: Medicine: Rehabilitation | Health Professions: Physical Therapy, Sports Therapy and Rehabilitation | Medicine: Orthopedics and Sports Medicine

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Category	Rank	Percentile
Medicine — Rehabilitation	#127/146	13th
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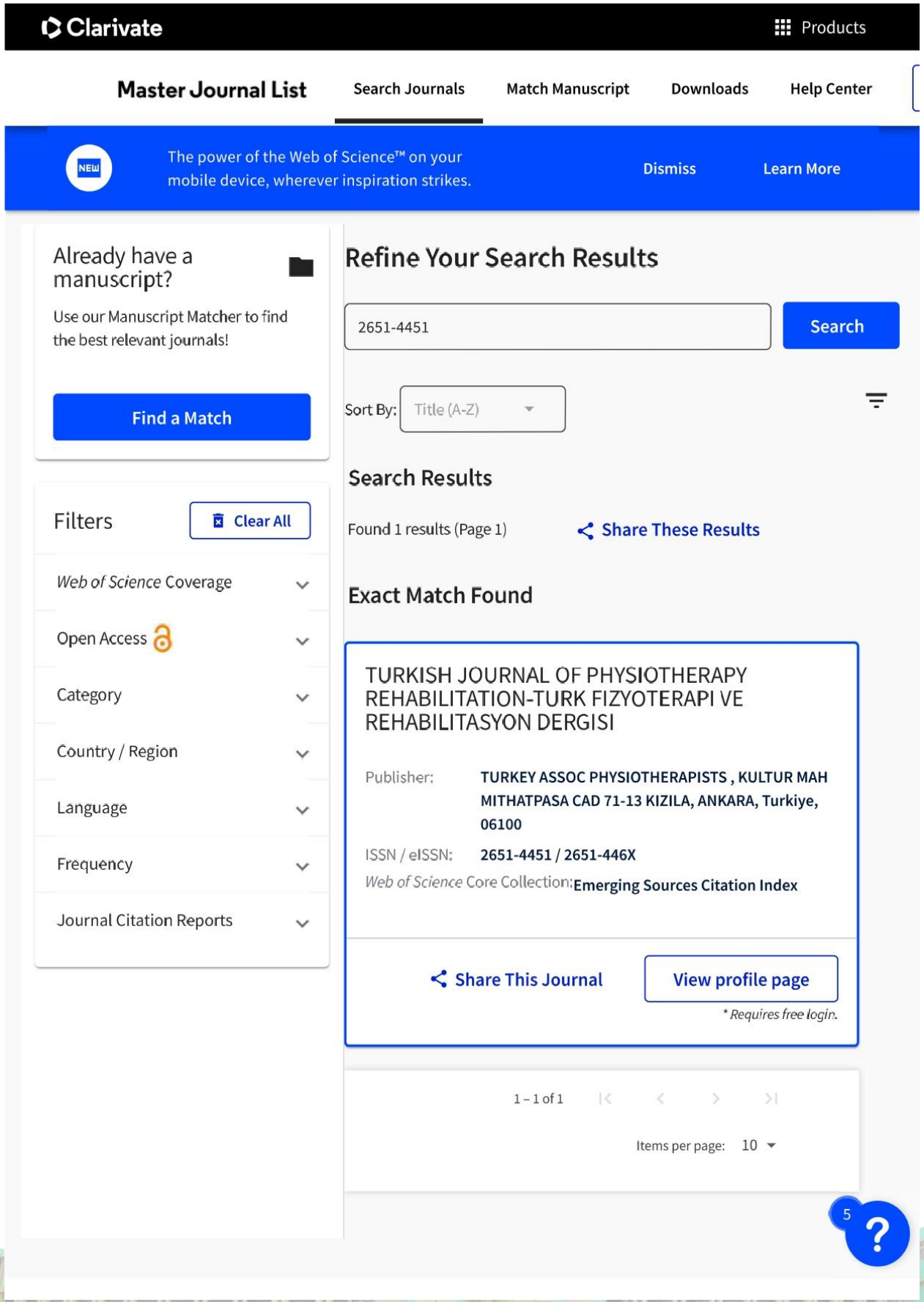
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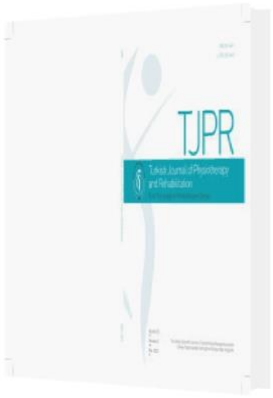

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ABOUT

Turkish Journal of Physiotherapy and Rehabilitation is the official peer-reviewed scientific journal of the Turkish Physiotherapy Association. It is abbreviated as Turk J Physiother Rehabil. The journal publishes three issues at April, August and December, in Turkish and English. This is a open access journal and all rights of the journal belongs toTurkish Physiotherapy Association.

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Turkish Journal of Physiotherapy and Rehabilitation; 32(2)
ISSN 2651-4451 | e-ISSN 2651-446X

FORMULATION OF VALUE-ADDED PRODUCTS FROM JAMUN SEED WITHOUT LOSS IN THE PHYSICOCHEMICAL AND MEDICAL PROPERTIES

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M.I. Niyas ahamed[5]
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[5]*Department of Biochemistry, Sacred Heart College (Autonomous), Tirupattur, Tamilnadu.*
[1]*Corresponding Author: dharshumaha@gmail.com*

ABSTRACT:

The aim of this study was to evaluate the physicochemical, proximate composition of Jamun (Syzygium Cumini) seed vitamins and minerals. The physical characteristics such as jamun color were registered as white to pink. The forms of the jamun seed were similar to the oblong forms. Jamun or Java plum seed was found to be long, wide and weight (18.20 mm, 11.05 mm and 1.62 g). Jamun seeds have been evaluated for their chemical composition as (53, 1.02, 3.84, 31.62, 7.01 and 1.51 g/100 g) such as moisture, crude fat, crude protein, carbohydrate or raw Fibres. The vitamin A (3 IU/100g), B3 (0.09 mg/100g) and C (0.21 mg/100g) presence values were recorded in jamun seed. Mineral values for jamun seed powder were iron, calcium, magnesium, phosphorus, potassium and zinc (0.140, 0.651,0.010, 0.072, 16.07 and 0.009 mg/100g). The conclusion was that the traditional medicinal plant seed jamun (*Syzygium Cumini*) provides a strong source of nutrients such as protein, fiber, vitamins, and minerals.

Keywords: Jamun fruits, Jamun seed, Physicochemical, Nutritional, Vitamin, Value Addition.

I. INTRODUCTION:

India is the source of many fruit cultivations and the majority of crops are confined to its growing area only. Their commercial production is lacking despite their high nutritional and medicinal properties. The majority of underused fruits are in many Ayurvedic formulations' core recipes. Jamun is the most common underused fruit that gains its popularity (Syzygium cumini). This species is native to Southeast Asia and India but has also been recorded as cultivated in Hawaii, Australia, Kenya, Florida, etc. The jamun fruits are grown annually and are available from June to July]. And jamun fruits are described as sweet savory berries. Kaatha, Narendra Jamun-6 and Konkan bhar doli are popular cultivars for jamun. The jamun fruit is a large berry, long-shaped and deep purple or bluish in colour. It has a purple pink pulp and a juicy fruit and a sweet fruit.

The world output of Jamun is estimated at 13.5 million tons annually, 15.4 percent of which was contributed by India. India is the second largest producer of Jamun in the world. In ayurvedic medicine, traditionally, jambul fruits, leaves, seeds and bark are used. For decades, Jamun seed powder has been used as a natural way to balance the amount of balanced blood sugar. It is a very tasty, detoxifying herb with properties to preserve normal urination and sweating. It has a hypolipidemic and cardioprotective immunomodulatory property. There are also studies on the antioxidant and radiation protection properties of the Jamun seed extract, as well as anti-inflammatory, anti-pyretic, anti-allergic, anti-bacterial and gastro-protective properties. It also works as a hepatic stimulant, digestive, cooling agent and blood purifier. Jamun seeds contain a glycoside, called jambolanas that helps to maintain glucose levels as normal. Ayurvedic text indicates that 1-3 g of jamun powder daily is an

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Saudi Journal of Biological Sciences

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Years currently covered by Scopus: From 2009 to 2024

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Subject area: Agricultural and Biological Sciences: General Agricultural and Biological Sciences

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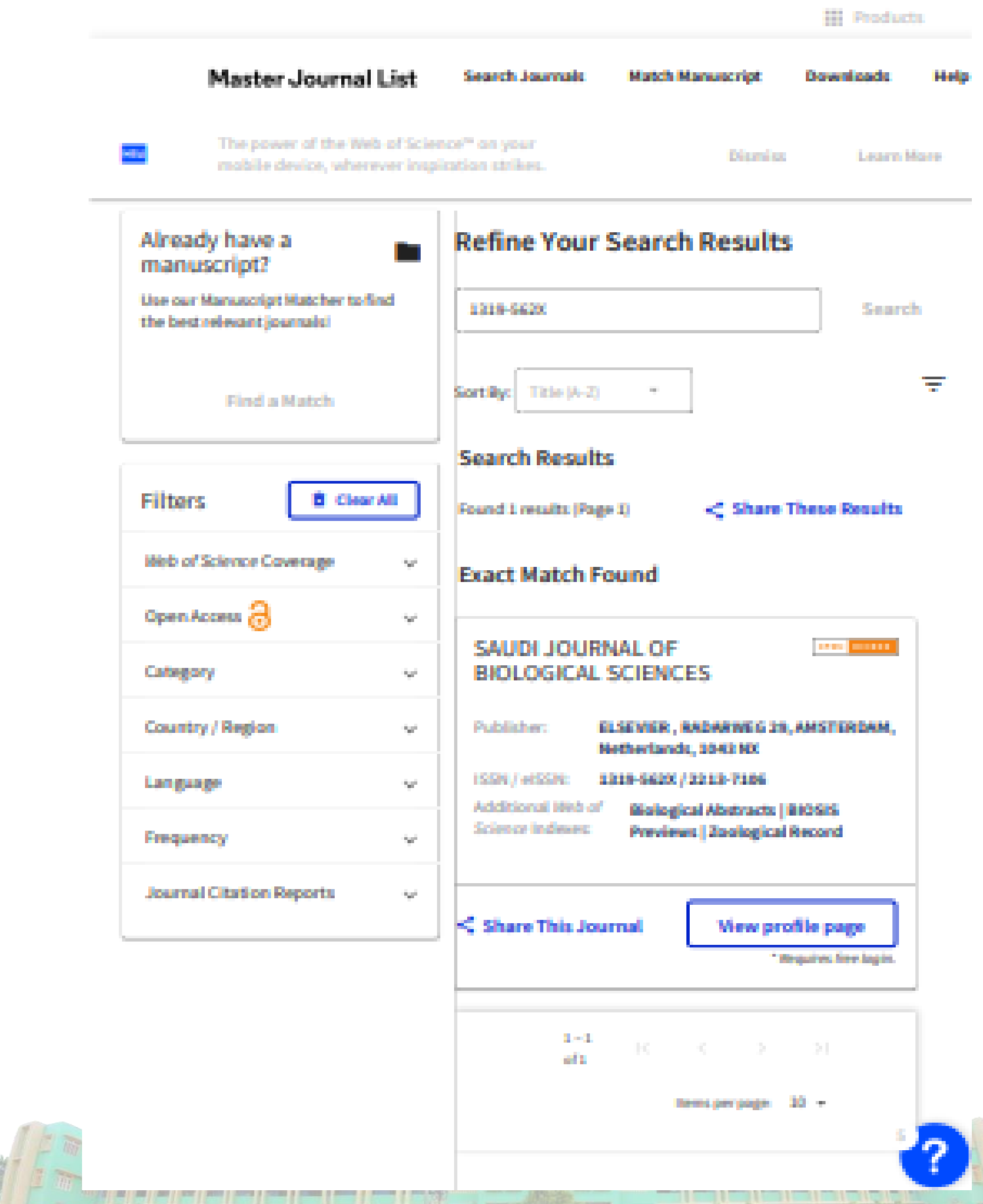
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Saudi Journal of Biological Sciences

Volume 28, Issue 8, August 2021, Pages 4117-4123

Original article

In vitro fibrinolytic activity of an enzyme purified from Bacillus amyloliquefaciens strain KJ10 isolated from *soybean paste*

Jayarajapasham Rajaselvam [a], Natarajan Benit [b], Saqer S. Alotaibi [c], M.A. Rathi [d], Sriramkaram Sriqopalram [e], Garupatham Devadhasan Biji [f], Ponnuswamy Vijayaraghavan [a]

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[c] Department of Biotechnology, College of Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia
[d] Department of Biochemistry, Sree Narayana Guru College, Coimbatore, Tamil Nadu 641 105, India
[e] Application Specialist, Genarem Biosciences Tiruchirapalli, Tamil Nadu 620021,India
[f] Department of Zoology, Nesamony Memorial Christian College, Marthandam, Kanyakumari, Tamil Nadu 629 165, India

Received 3 March 2021, Revised 22 April 2021, Accepted 22 April 2021, Available online 1 May 2021, Version of Record 21 July 2021.

https://doi.org/10.1016/j.sjbs.2021.04.061

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Source details

Journal of Infection and Public Health

Open Access

Years currently covered by Scopus: from 2008 to 2024

Publisher: Elsevier

ISSN: 1876-0341 E-ISSN: 1876-0358

Subject area: Medicine: Public Health, Environmental and Occupational Health; Medicine: Infectious Diseases

Source type: Journal

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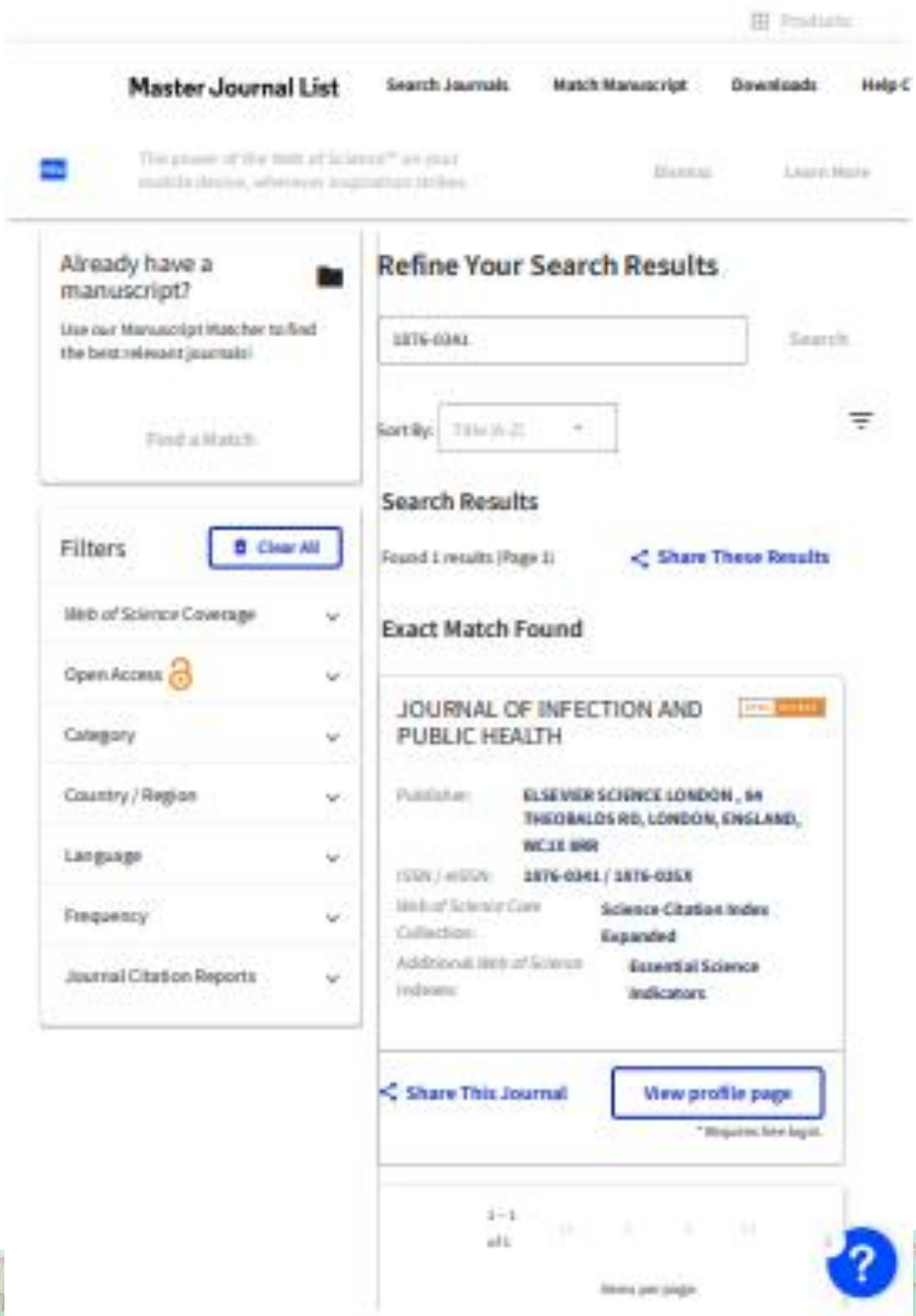
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Journal of Infection and Public Health

Volume 14, Issue 7, July 2021, Pages 890-897

Carbapenemases producing *Klebsiella pneumoniae* from the pus of hospitalized patients: In-vitro antibiotic properties of *Streptomyces* against multidrug resistant infectious bacteria

Balamuralikrishnan Balasubramanian [a], Natarajan Benit [b], Paul Agastian [c], Khalid S. Almaary [d], Turki M. Dawoud [d], Yahya B. Elbadawi [d], Ayman Mubarak [d], Mohammed S. Alfadul [d], Reem M. Aljowaie [d]

[a] Department of Food Science and Biotechnology, College of Life Science, Sejong University, Seoul 05006, South Korea

[b] Department of Botany, Holy Cross College, ManonmaniamSundaranar University, Abishekapatti, Tirunelveli 627 012, Tamil Nadu, India

[c] Research Department of Plant Biology and Biotechnology, Loyola College, Chennai, Tamil Nadu, India

[d] Department of Botany and Microbiology, College of Science, King Saud University, P.O. 2455, Riyadh 11451, Saudi Arabia

Received 15 February 2021, Revised 10 May 2021, Accepted 18 May 2021, Available online 27 May 2021, Version of Record 11 June 2021.

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E-ISSN: 2214-7853

Subject area: Materials Science: General Materials Science

Source type: Conference Proceeding

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Materials Today: Proceedings

Volume 45, Part 2, 2021, Pages 2087-2090

Production and characterization of extracellular pectinase from a newly isolated Bacillus species from fruit waste soil

T. Murugan [a], P. Deepika [a], A. Kowsalya [a], K. Sivasubramanian [a], R.P. Rejisha [b], M. Murugan [b], J. Albino Wins [c]

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https://doi.org/10.1016/j.matpr.2020.09.607

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Abstract

The present investigation was carried for identification of pectinolytic bacteria and determination of their pectinolytic activity. The isolation was made from soil sample collected from fruit wastes. Screening of pectinolytic activity was achieved with pectin agar plate. Among 36 strains tested 12 shows pectinolytic activity. The potent isolate FWS II-4 was identified as *Bacillus* sp. and further used for enzyme production. Pectinase was produced by submerged fermentation and the purified. The purified enzyme demonstrated 3.40 mg/ml of total protein and 484.70 U/mg of specific activity. In characterization studies, the pectinase demonstrated good activity at pH 6.0 and 40 °C. Also, the bacterial strain showed maximum growth when the medium pH was 7.0 and incubated 37 °C.

Introduction

Pectin is large molecular weight polysaccharides that are commonly found in plants [1], [2], [3]. Pectinase is a complex of enzymes involved in the biological degradation of pectin [4]. Polygalacturonase is commercially used pectinase that cleave the glycosidic bonds present in the of galaturonic acid [5]. The pectinolytic enzymes have been classified into depolymerases, esterases and protopectinases [4], [6]. Pectinases are important in plants for fruit ripening, signaling and cell adhesion [7], [8].

Pectinase possess significant industrial importances that are used in the production of fruit juices, wines and vegetable oil [9], [10], [11]. It has remarkable applications in food, pharmaceutical, textile industry [12] and fruit juice wastewater treatment [13].

In global food enzyme sales, pectinases are accounts for approximately 25% [11] and 10% of the global industrial enzyme production [14]. Pectinases have been produced by many organisms include plants, nematodes, insects, bacteria, fungi mold, yeast, actinomycetes and protozons [15]. The majority of pectinases are produced by bacteria [16], fungi [17] and actinomycetes [18]. The bacterial isolates that are producing industrially important pectinase are including the bacterial genera such as *Bacillus*, *Pseudomonas* and *Staphylococcus* [18], [19]. Among these, *Bacillus* species has the significances to produce pectinase in large quantities [13], [20]. The study aimed to identify pectinolytic bacteria in fruit waste soil and study the characteristics of enzyme and bacterial isolate for obtaining commercially importance pectinase with high activity.

Section snippets

Soil sample

Fruit waste soil was collected in and around Arakkonam market area situated in Ranipet district, Tamil Nadu, India. The

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Linguistica Antverpiensia, New Series – Themes in Translation Studies

Scopus coverage years: from 2002 to 2023

Publisher: Department of Applied Linguistics, Translators and Interpreters, University of Antwerp

ISSN: 0304-2294 E-ISSN: 2295-5739

Subject area: Arts and Humanities: Language and Linguistics | Social Sciences: Linguistics and Language

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Social Sciences Linguistics and Language	#218/1078	79th

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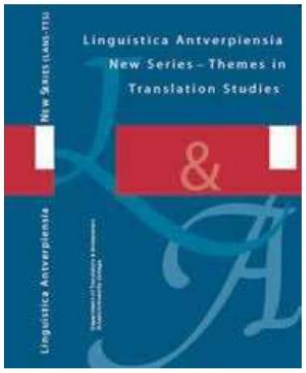

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Guest editors

- **Lu Xinchao, Beijing Foreign Studies University (China)**
- **Claudio Fantinuoli, Mainz University (Germany)**

Practical information and deadlines

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Function of Brain in L2 Learning - Neurolinguistic Perspective

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Abstract

Language learning is a basic concept of all over the world. To learn a foreign language, there should be proper guidance and proper coaching. The students should know the rules and principles which are followed by the native speakers. L2 learning is not an easy task, at first all grammatical rules and the phonetics have to be taught to the learners. There are several methods which are used for training an individual in English. Grammar Translation method is the pioneer method which is followed in 19th century. After few years, Bilingual method, Translation method, Eclectic method are introduced for foreign language teaching. All these methods are completely formal and focus upon direct learning and teaching process. These methods are formal and boring so that there is a lot of chance for the students to get deviated from learning. Grammatical rules and syntax are boring part in a language study. So there should be a better method for learning a language. The present generation focuses on Neuro science as

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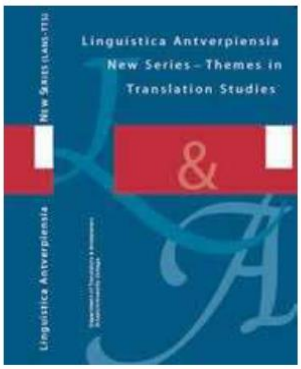

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The Prominence of Innovative Ideas and Technologies in ELT Classroom

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Abstract

Learning English language is entirely basic for making opportunities. English as it is known, is a worldwide language which makes a simple access with various tongues of the world. Learning English language keeps away from false impressions in language development and communication process. The role of innovation in learning English language through cooperation would clear away boundaries in complete comprehension of feelings. Human language can be verbal or non-verbal that passes on feelings. Everything is identified with human feelings, which can be passed on through language. Language is a scholarly mine where an individual can discover supportive for the basic living. It could be productivity and displacement, and depends totally on social show and learning. People secure language through social collaboration in early adolescence and youngsters by and large smoothly. This paper focuseson the degree of utilizing inventive showing