Nandurbar Taluka Vidhayak Samiti's
G. T. PATIL ARTS COMMERCE AND SCIENCE COLLEGE, NANDURBAR – 425412
NAAC ACCREDITED 'A' GRADE
(Affiliated to Kavayitri Bahinabai Chaudhari North Maharashtra University, Jalgaon)

Prof. Dr. M.J. Raghuwanshi
I/Principal

Email: gtpcollege@rediffmail.com
Ph: 2564-222293
Website: ntvsgtpcollege.org

Date: 10-05-2023

Declaration

This is to inform that information, reports, true copies of the supporting documents, numerical data etc. submitted/ presented in this file is verified by Internal Quality Assurance Cell (IQAC) and is correct as per the records. This declaration is for the purpose of NAAC Accreditation of HEI for Third Cycle period 2017-18 to 2021-22.

Date:10-05-2023
Place: Nandurbar

Dr.V.Z.Chaudhari
Co-ordinator,IQAC
GTP College,Nandurbar

(Prof. Dr. M.J Raghuwanshi)
PRINCIPAL
GT Patil College,
Nandurbar-425412

3.2.1 Institution has created an ecosystem for innovations and has initiatives for creation and transfer of knowledge (patents filed, published, incubation centre facilities in the HEI *to be considered)*

Being the oldest college, the college has commitment to fulfil the needs of rural and deprived sections of society in terms of knowledge, innovations, and scientific solutions to their lifelong problems. The institutional ecosystem is helping to nurture innovative and creative ideas by developing research-oriented skills.

Sr. No.	Activity
1	KIED Cell
2	Research Guides
3	Patents
4	MoU/ Collaboration
5	Webinar

Dr.V.Z.Chaudhari
Co-ordinator,IQAC
GTP College,Nandurbar

(Prof. Dr. M.J Raghuwanshi)
PRINCIPAL
GT Patil College,
Nandurbar-425412

KIEDC Cell

Nandurbar Taluka Vidhayak Samiti's
G. T. PATIL ARTS COMMERCE AND SCIENCE COLLEGE,
NANDURBAR - 425412
NAAC ACCREDITED 'A' GRADE
(Affiliated to KBC, North Maharashtra University, Jalgaon)

Prof. V. S. Shrivastava
Principal

Email: gtpcollege@rediffmail.com
Ph: 2564-222293
Website: ntvsgtpcollege.org

INCUBATION / KIED CELL

2021-22

Information of Incubation/K-IEDC.

KCIIL-Innovation and Entrepreneur Development Cell (K-IEDC) is established at Nandurbar Taluka Vidhayak Samiti's G. T. Patil Arts, Commerce and Science College, Nandurbar. It is working in collaboration with Kavayitri Bahinabai Chaudhari North Maharashtra University Centre for Innovation, Incubation and Linkages (KCIIL). Its aim is to build knowledge innovation ecosystem to solve the societal problems by adapting effective scientific approaches and to encourage to set-up startups via college ecosystem.

Objectives:

- To develop active knowledgeable start-up ecosystem
- To encourage faculties and students to participate in advance scientific programs to achieve desirable outcomes of mutual growth.
- To establish contacts with local small scale entrepreneurs and help them to grow by solving the issues through consultation.
- Entrepreneurship promotion through Self-Employment and Talent Utilization, wherein innovators would be supported and mentored to become successful entrepreneurs.
- To spread awareness about scientific innovations and their benefit in day-to-day life.
- To explore entrepreneurship opportunities through K-IEDC.

Functions:

- It provides incubation infra supports to students and researchers.
- It offers specialized facilities to the society.
- It makes grant management of the different research /startup.
- It provides technical and business mentoring support to entrepreneurs.
- It comes with Patent and IPR support to students and researchers.

We are committed to run this cell effectively through arrangement of following thing:

- Sessions of successful entrepreneurs or startup founders
- Session on process of innovation development, intellectual
- Arrangement of workshop or seminar on various innovations

COMMITTEE

Sr. No.	Name of member	Structure
1	**Prof. V. S Shrivastava**	**Principal**
2	**Dr. M. R Patil**	**Coordinator**
3	**Dr. G R Gupta**	**Member**
4	**Dr A N Kulkarni**	**Member**
5	**Marathe Sakshi Pratap**	**Member**
6	**Patil Suvarna Santosh**	**Member**
7	**Borse Akshay Dnyaneshwar**	**Member**
8	**Patil Purshottam Sanjay**	**Member**
9	**Raghuwanshi Aditya Vinod**	**Member**
10	**Tamboli Pushpendra Pramod**	**Invitee Member**
11	**Dr Rajput Chetan Vijaysing**	**Invitee Member**

(Prof. Dr. V. S. Shrivastava)
Principal

PRINCIPAL
G.T.Patil Arts,Commerce &
Science College
NANDURBAR - 425 412 (M.S.)

Research Guides

Nandurbar Taluka Vidhayak Samiti's
G. T. PATIL ARTS COMMERCE AND SCIENCE COLLEGE,
NANDURBAR – 425412
NAAC ACCREDITED 'A' GRADE
(Affiliated to KBC North Maharashtra University, Jalgaon)

Prof. M. J. Raghuwanshi
M.A. Ph.D.
Principal

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Website: ntvsgtpcollege.org

Date: 08/05/2023

List of Ph. D. Guides

Sr No	Name of the Research Guide	Subject	Guideship Letter No.	Date
1	Dr M J Raghuwanshi	Hindi	KBCNMU/11/PGR/Hindi/6001/2011	Date :5.12.2011
2	Dr. P. A. Bhamare	Marathi	NMU/11/PGR/Marathi/ 2196/ 2010	Date : 01.09.2010
3	Dr A M Pawar	Hindi	KBCNMU/11/PGR/Hindi/2433/2012	Date :25.09.2012
4	Dr V S Patil	Marathi	KBCNMU/11/PGR//Marathi/2276/2013	Date : 14.11.2013
5	Dr M K Kadam	Marathi	KBCNMU/11/PGR/Marathi/2284/2013	Date : 14.11.2013
6	Dr S B Wayse	Economics	KBCNMU/11/PGR/Economics/2317/2013	Date 14.11.2013
7	Dr P K Gautam	Botany	KBCNMU/11/PGR/Bot/2324/2013	Date 12.11.2013
8	Dr D D Girase	English	KBCNMU/11/PGR/624/2018	Date : 30.01.2018
9	Dr G H Balde	Zoology	KBCNMU/11/PGR/Zoo/2098/2019	Date:20.05.2019
10	Dr V Z Chaudhari	English	KBCNMU/11/PGR/Eng/2123/2019	Date : 29.05.2019
11	Dr N B Shende	History	KBCNMU/11/PGR/his/2415/2019	Date : 29.05.2019
12	Dr Sameera Ahmad	Botany	KBCNMU/11/PGR/Bot/5106/2019	Date :11.12.2019
13	Dr S R Surye	Psychology	KBCNMU/11/PGR/Psy/555/2020	Date :28.01.2020
14	Dr Manohar R Patil	Chemistry	KBCNMU/11/PGR/Chemistry/1515/2020	Date :20.05.2020
15	Dr Amol Bhuyar	Geography	KBCNMU/11/PGR/Geo/1483/2020	Date 20.05.2020
16	Dr T L Das	Physical Ed.	KBCNMU/11/PGR/Phy.edu/2327/2020	Date:27.08.2020
17	Dr Gaurav Gupta	Chemistry	KBCNMU/11/PGR/Chemistry/1518/2020	Date : 20.05.2020
18	Dr Anil Kulkarni	Physics	KBCNMU/11/PGR/Phy/1478/2020	Date :20.05.2020
19	Dr. V. V. Patil	History	KBCNMU/11/PGR/His/ 2287/2022	Date: 24.08.2020
20	Dr. P.S . Patil	Chemistry	KBCNMU/11/Ph.D./ 10 /2022	Date: 2.08.2022
21	Dr V G Somkuwar	History	KBCNMU/11/PGR/Phy.Edu/167/2022	Date: 2.08.2022
22	Dr. S P Patil	Chemistry	KBCNMU/11/Ph.D./ 27 /2022	Date: 2.08.2022
23	Dr D B Deore	English	KBCNMU/11/Ph.D./ 21 /2022	Date: 2.08.2022
24	Dr M S Waghmare	Political Science	KBCNMU/11/Ph.D./ 145 /2022	Date: 2.08.2022
25	Dr S U Ahire	Psychology	KBCNMU/11/Ph.D./ 149 /2022	Date: 2.08.2022
26	Dr. N P Huse	Physics	KBCNMU/11/Ph.D./ 69 /2022	Date: 2.08.2022
27	Dr R R Deore	Geography	KBCNMU/11/Ph.D./30/2022	Date: 2.08.2022
28	Dr S V Mishra	Commerce	KBCNMU/11/Ph.D./ 196 /2022	Date: 2.08.2022
29	Dr D S Patil	Zoology	KBCNMU/11/Ph.D./ 56 /2022	Date: 2.08.2022
30	Dr Y V Marathe	Chemistry	KBCNMU/11/Ph.D./ 121 /2022	Date: 2.08.2022
31	Dr. V.F. Makrani	Hindi	KBCNMU/11/Ph.D./ 122/2022	Date: 2.08.2022
32	Dr. S. P. Pawar	Marathi	KBCNMU/11/Ph.D./ 141/2022	Date: 2.08.2022
33	Dr.U. J. Dhagdhage	Defence Studies	KBCNMU/11/Ph.D/335/2022	Date: 4.08.2022

(Prof. Dr. M.J.Raghuwanshi)

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Nandurbar-425412

Patents

पेटेंट कार्यालय
शासकीय जर्नल

OFFICIAL JOURNAL
OF
THE PATENT OFFICE

निर्गमन सं. 18/2022	शुक्रवार	दिनांक: 06/05/2022
ISSUE NO. 18/2022	**FRIDAY**	**DATE: 06/05/2022**

पेटेंट कार्यालय का एक प्रकाशन

PUBLICATION OF THE PATENT OFFICE

INTRODUCTION

In view of the recent amendment made in the Patents Act, 1970 by the Patents (Amendment) Act, 2005 effective from 01st January 2005, the Official Journal of The Patent Office is required to be published under the Statute. This Journal is being published on weekly basis on every Friday covering the various proceedings on Patents as required according to the provision of Section 145 of the Patents Act 1970. All the enquiries on this Official Journal and other information as required by the public should be addressed to the Controller General of Patents, Designs & Trade Marks. Suggestions and comments are requested from all quarters so that the content can be enriched.

(PROF. (DR) UNNAT P. PANDIT)
CONTROLLER GENERAL OF PATENTS, DESIGNS & TRADE MARKS

06TH MAY, 2022

CONTENTS

(12) PATENT APPLICATION PUBLICATION
(19) INDIA
(22) Date of filing of Application :30/04/2022

(21) Application No.202211025461 A
(43) Publication Date : 06/05/2022

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(54) Title of the invention : A SYSTEM & METHOD FOR RAIL TRANSPORTATION PROPERTY MANAGEMENT USING AI & ML

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(51) International classification	:G06Q0010060000, G06Q0050160000, G06Q0050180000, G06Q0010000000, G06Q0010100000
(86) International Application No Filing Date	:NA :NA
(87) International Publication No	: NA
(61) Patent of Addition to Application Number Filing Date	:NA :NA
(62) Divisional to Application Number Filing Date	:NA :NA

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4)Madan Mohan Gupta
5)Kannadasan B
6)ASHIQ V M
7)Rupesh Ramesh Deore
8)Ankit Kumar Navalakha
9)Harpreet Singh Bedi
10)Deo Karan Ram
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	Address of Applicant :Assistant professor, Department school of electronics and electrical engineering Lovely professional University, Punjab ----------- ----------- **10)Deo Karan Ram** Address of Applicant :Associate Professor, Petroleum and Chemical Engineering, NIMS University Rajasthan, Jaipur ----------- ----------- **11)Ankit Jain** Address of Applicant :Research Scholar, Amity University, Jaipur, Rajasthan ----------- ----------- **12)Priyanka Aggarwal** Address of Applicant :A2Z Softech, Ghaziabad ----------- -----------

(57) Abstract :

The present invention is artificial intelligence and the machine learning-based railway assessment management system. The scope of the criteria covers key aspects of rail Property management systems including Property performance management like operations and maintenance, condition and reliability monitoring, and Property management business processes. It also includes general product functions, Property types, deployment strategies, work order management, materials management, labour management, service contract management, financial management, reporting and analytics, and technology architecture. The present invention is very much useful in developing countries like India where so much amount of the government is spent on railways. In such scenarios, this invention works as a guide, has attributes tailored for rail operators and transit agencies and allows those involved in a rail Property management selection process to make improved decisions more quickly. The key metrics of the present railway assessment management invention is the overall maintenance which involves uptime, Property longevity, cost control, and safety across a diverse set of Properties and technologies. The system works as a total solution, that has become complex and functionality involves the combination of an expanded range of capabilities and specific technology requirements. The details are discussed in the figures of the invention.

No. of Pages : 27 No. of Claims : 7

ORIGINAL

मूल/No : 126785

भारत सरकार
GOVERNMENT OF INDIA
पेटेंट कार्यालय
THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No. : 370337-001

तारीख / Date : 03/09/2022

पारस्परिकता तारीख / Reciprocity Date* :

देश / Country :

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **DEVICE TO PERFORM ANALYSIS OF POLYMER CONCRETE** से संबंधित है, का पंजीकरण, श्रेणी **10-05** में 1.Gomadurai Chinnasamy 2. Venkatesa Prabhu Sundramurthy 3.Rajan Pratihast 4.Dr. Manohar Rajendra Patil के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **10-05** in respect of the application of such design to **DEVICE TO PERFORM ANALYSIS OF POLYMER CONCRETE** in the name of 1.Gomadurai Chinnasamy 2. Venkatesa Prabhu Sundramurthy 3.Rajan Pratihast 4.Dr. Manohar Rajendra Patil.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।

In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

निर्गमन की तारीख/Date of Issue : 23/01/2023

महानियंत्रक पेटेंट डिजाइन और व्यापार चिह्न
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पारस्परिकता तारीख (यदि कोई हो) जिसकी अनुमति देश के नाम पर की गई है। डिजाइन का सत्त्वाधिकार पंजीकरण की तारीख से दस वर्षों के लिए होगा जिसका विस्तार, अधिनियम एवं नियम के निबंधनों के अधीन, पाँच वर्षों की अतिरिक्त अवधि के लिए किया जा सकेगा। इस प्रमाण पत्र का उपयोग विधिक कार्यवाहियों अथवा विदेश में पंजीकरण प्राप्त करने के लिए नहीं हो सकता है।

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ORIGINAL

मूल/No : 124873

सत्यमेव जयते

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THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No.	:	364927-001
तारीख / Date	:	26/05/2022
पारस्परिकता तारीख / Reciprocity Date*	:	
देश / Country	:	

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **SMART ANIMAL WEARABLE DEVICE TO IDENTIFY POLLUTION** से संबंधित है, का पंजीकरण, श्रेणी **10-05** में Dr. Manohar Rajendra Patil के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **10-05** in respect of the application of such design to **SMART ANIMAL WEARABLE DEVICE TO IDENTIFY POLLUTION** in the name of Dr. Manohar Rajendra Patil.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।

In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

निर्गमन की तारीख/Date of Issue : 12/01/2023

महानियंत्रक पेटेंट डिजाइन और व्यापार चिह्न
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ORIGINAL

मूल/No : 125596

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THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No. : 367370-001

तारीख / Date : 07/07/2022

पारस्परिकता तारीख / Reciprocity Date* :

देश / Country :

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **ROBOTIC DEVICE FOR PEST CONTROL IN FARM** से संबंधित है, का पंजीकरण, श्रेणी **15-03** में 1.Dr. Prakash Tanaji Wankhedkar 2. Mr. Dilip Haribhau Dudhmal 3.Dr. Prashant Kantilal Bagul 4.Dr. Dhananjay Shivajirao Patil के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **15-03** in respect of the application of such design to **ROBOTIC DEVICE FOR PEST CONTROL IN FARM** in the name of 1.Dr. Prakash Tanaji Wankhedkar 2. Mr. Dilip Haribhau Dudhmal 3.Dr. Prashant Kantilal Bagul 4.Dr. Dhananjay Shivajirao Patil.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।

In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

निर्गमन की तारीख/Date of Issue : 16/01/2023

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*The reciprocity date (if any) which has been allowed and the name of the country.Copyright in the design will subsist for ten years from the date of Registration, and may under the terms of the Act and Rules, be extended for a further period of five years.This Certificate is not for use in legal proceedings or for obtaining registration abroad.

ORIGINAL

मूल/No : 125357

सत्यमेव जयते

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THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No.	:	373525-001
तारीख / Date	:	03/11/2022
पारस्परिकता तारीख / Reciprocity Date*	:	
देश / Country	:	

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **ELECTROCARDIOGRAM DETECTING VEST** से संबंधित है, का पंजीकरण, श्रेणी **24-04** में 1.Dr. Prakash Tanaji Wankhedkar 2. Dr. Dhananjay Shivajirao Patil 3.Dr. Prashant Kantilal Bagul के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **24-04** in respect of the application of such design to **ELECTROCARDIOGRAM DETECTING VEST** in the name of 1.Dr. Prakash Tanaji Wankhedkar 2. Dr. Dhananjay Shivajirao Patil 3.Dr. Prashant Kantilal Bagul.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।

In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

निर्गमन की तारीख/Date of Issue : 13/01/2023

महानियंत्रक पेटेंट डिजाइन और व्यापार चिह्न
Controller General of Patents, Designs and Trade Marks

पारस्परिकता तारीख (यदि कोई हो) जिसकी अनुमति देश के नाम पर की गई है। डिजाइन का सत्त्वाधिकार पंजीकरण की तारीख से दस वर्षों के लिए होगा जिसका विस्तार, अधिनियम एवं नियम के निबंधनों के अधीन, पाँच वर्षों की अतिरिक्त अवधि के लिए किया जा सकेगा। इस प्रमाण पत्र का उपयोग विधिक कार्यवाहियों अथवा विदेश में पंजीकरण प्राप्त करने के लिए नहीं हो सकता है।

*The reciprocity date (if any) which has been allowed and the name of the country.Copyright in the design will subsist for ten years from the date of Registration, and may under the terms of the Act and Rules, be extended for a further period of five years.This Certificate is not for use in legal proceedings or for obtaining registration abroad.

(12) PATENT APPLICATION PUBLICATION
(19) INDIA
(22) Date of filing of Application :13/10/2022
(21) Application No.202241058657 A
(43) Publication Date : 18/11/2022

(54) Title of the invention : INNOVATION IN EDUCATIONAL MARKETING TO PRIVATE HIGHER EDUCATION INSTITUTIONS & METHODS THEREOF

(51) International classification	:G06Q0030020000, G06Q0010060000, G06Q0050200000, G06Q0010100000, G09B0019000000
(86) International Application No Filing Date	:PCT// :01/01/1900
(87) International Publication No	: NA
(61) Patent of Addition to Application Number Filing Date	:NA :NA
(62) Divisional to Application Number Filing Date	:NA :NA

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(57) Abstract :

ABSTRACT INNOVATION IN EDUCATIONAL MARKETING TO PRIVATE HIGHER EDUCATION INSTITUTIONS & METHODS THEREOF The present disclosure relates to a method of innovation in educational marketing to private higher education institutions. It makes sense that the quality of human capital and the effectiveness of its use depend on the quantity and quality of individual labor invested in the process of consuming educational services, as well as on one's own abilities, the extent to which those abilities are realized, and other subjective factors. The study's goal is to investigate how to enhance the marketing of educational services using a cutting-edge strategy. Analysis of new marketing strategies for educational services, evaluation of the product's level of competition, and public-private administration of education. The study's goal is to investigate how to enhance the marketing of educational services using a cutting-edge strategy. Analysis of new marketing strategies for educational services, evaluation of the product's level of competition, and public-private administration of education. It has been found that using educational services results in the creation of human capital.

No. of Pages : 19 No. of Claims : 6

सत्यमेव जयते

ORIGINAL

मूल/No : 127411

भारत सरकार
GOVERNMENT OF INDIA
पेटेंट कार्यालय
THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No.	:	375714-001
तारीख / Date	:	16/12/2022
पारस्परिकता तारीख / Reciprocity Date*	:	
देश / Country	:	

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **DEVICE TO DETECT HEMOSTATIC FUNCTION IN ANIMALS** से संबंधित है, का पंजीकरण, श्रेणी **24-01** में 1.Dr. Sangeeta Bhimrao Dongre 2. Dr. Dhananjay Shivajirao Patil 3.Dr. Prakash Tanaji Wankhedkar के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **24-01** in respect of the application of such design to **DEVICE TO DETECT HEMOSTATIC FUNCTION IN ANIMALS** in the name of 1.Dr. Sangeeta Bhimrao Dongre 2. Dr. Dhananjay Shivajirao Patil 3.Dr. Prakash Tanaji Wankhedkar.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।
In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

निर्गमन की तारीख/Date of Issue : 25/01/2023

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*The reciprocity date (if any) which has been allowed and the name of the country.Copyright in the design will subsist for ten years from the date of Registration, and may under the terms of the Act and Rules, be extended for a further period of five years.This Certificate is not for use in legal proceedings or for obtaining registration abroad.

ORIGINAL

मूल/No : 132225

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THE PATENT OFFICE
डिजाइन के पंजीकरण का प्रमाणपत्र
CERTIFICATE OF REGISTRATION OF DESIGN

डिजाइन सं. / Design No.	:	367697-001
तारीख / Date	:	14/07/2022
पारस्परिकता तारीख / Reciprocity Date*	:	
देश / Country	:	

प्रमाणित किया जाता है कि संलग्न प्रति में वर्णित डिजाइन जो **GLASS TO IDENTIFY THE QUANTITY OF SUGAR AND CALORIE IN FOOD** से संबंधित है, का पंजीकरण, श्रेणी **10-05** में 1.Dr. Prakash Tanaji Wankhedkar 2. Dr. Bhaskar Chandu More 3.Dr. Dhananjay Shivajirao Patil 4.Dr. Shaikh Hasim Mohammed Isak के नाम में उपर्युक्त संख्या और तारीख में कर लिया गया है।

Certified that the design of which a copy is annexed hereto has been registered as of the number and date given above in class **10-05** in respect of the application of such design to **GLASS TO IDENTIFY THE QUANTITY OF SUGAR AND CALORIE IN FOOD** in the name of 1.Dr. Prakash Tanaji Wankhedkar 2. Dr. Bhaskar Chandu More 3.Dr. Dhananjay Shivajirao Patil 4.Dr. Shaikh Hasim Mohammed Isak.

डिजाइन अधिनियम, 2000 तथा डिजाइन नियम, 2001 के अध्यधीन प्रावधानों के अनुसरण में।
In pursuance of and subject to the provisions of the Designs Act, 2000 and the Designs Rules, 2001.

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महानियंत्रक पेटेंट डिजाइन और व्यापार चिह्न
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पारस्परिकता तारीख (यदि कोई हो) जिसकी अनुमति देश के नाम पर की गई है। डिजाइन का सत्त्वाधिकार पंजीकरण की तारीख से दस वर्षों के लिए होगा जिसका विस्तार, अधिनियम एवं नियम के निबंधनों के अधीन, पाँच वर्षों की अतिरिक्त अवधि के लिए किया जा सकेगा। इस प्रमाण पत्र का उपयोग विधिक कार्यवाहियों अथवा विदेश में पंजीकरण प्राप्त करने के लिए नहीं हो सकता है।

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ISSUE NO. 52/2022	**FRIDAY**	**DATE: 30/12/2022**

पेटेंट कार्यालय का एक प्रकाशन
PUBLICATION OF THE PATENT OFFICE

(12) PATENT APPLICATION PUBLICATION
(21) Application No.202211071696 A
(19) INDIA
(22) Date of filing of Application :12/12/2022
(43) Publication Date : 30/12/2022

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(54) Title of the invention : ARTIFICIAL INTELLIGENCE BASED APPROACH TO PREDICT THE FACTORS RESPONSIBLE FOR CONTAMINATION OF FOOD CHAIN THROUGH UNCERTAINTY MODELLING

(51) International classification :H01L0021670000, G06F0030200000, A61B0005145000, A23B0004220000, A23L0003346300
(86) International Application No :NA
Filing Date :NA
(87) International Publication No : NA
(61) Patent of Addition to Application Number :NA
Filing Date :NA
(62) Divisional to Application Number :NA
Filing Date :NA

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(57) Abstract :
Artificial Intelligence based approach to Predict the factors responsible for contamination of food chain through uncertainty modelling is the proposed invention. The proposed invention focuses on predicting the factors responsible for causing contamination of food. The invention aims at utilizing the algorithm so uncertainty modelling for analyzing the contaminants that are present in the food.

No. of Pages : 13 No. of Claims : 6

(12) PATENT APPLICATION PUBLICATION
(19) INDIA
(22) Date of filing of Application :22/08/2022
(21) Application No.202241047668 A
(43) Publication Date : 23/09/2022

(54) Title of the invention : MACHINE LEARNING BASED APPROACH TO CLASSIFY THE TYPES OF BLOOD CANCERS BASED ON THE BLOOD COMPOSITION AND ITS STRUCTURE

(51) International classification	:A61B0005145000, G01N0015140000, A61B0005000000, G06N0020000000, A61B0005145500
(86) International Application No	:PCT//
Filing Date	:01/01/1900
(87) International Publication No	: NA
(61) Patent of Addition to Application Number	:NA
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(62) Divisional to Application Number	:NA
Filing Date	:NA

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(57) Abstract :
Machine Learning based approach to Classify the Types of Blood Cancers based on the Blood Composition and Its Structure is the proposed invention. The proposed invention focuses on identifying the type of blood cancer using the blood composition report. The algorithms of machine learning is used predict the exact condition by analyzing the blood structure as well. The invention aims at understanding the condition and stage of blood cancer and pave way for precise treatment.

No. of Pages : 15 No. of Claims : 6

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पेटेंट कार्यालय का एक प्रकाशन
PUBLICATION OF THE PATENT OFFICE

(12) PATENT APPLICATION PUBLICATION
(19) INDIA
(22) Date of filing of Application :12/12/2022

(21) Application No.202211071696 A
(43) Publication Date : 30/12/2022

(54) Title of the invention : ARTIFICIAL INTELLIGENCE BASED APPROACH TO PREDICT THE FACTORS RESPONSIBLE FOR CONTAMINATION OF FOOD CHAIN THROUGH UNCERTAINTY MODELLING

(51) International classification	:H01L0021670000, G06F0030200000, A61B0005145000, A23B0004220000, A23L0003346300
(86) International Application No	:NA
Filing Date	:NA
(87) International Publication No	: NA
(61) Patent of Addition to Application Number	:NA
Filing Date	:NA
(62) Divisional to Application Number	:NA
Filing Date	:NA

(71)**Name of Applicant :**
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7)MUHAMMAD RIZWAN TARIQ
8)SWAPNIL SAURAV
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10)Dr.A.SASI KUMAR
11)AJAY DUREJA
12)Dr. SACHIN SABHARWAL
Name of Applicant : NA
Address of Applicant : NA
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8)SWAPNIL SAURAV
Address of Applicant :RESEARCH SCHOLAR, DEPARTMENT OF COMPUTER SCIENCE AND ENGINEERING, GITAM UNIVERSITY, RUDRARAM,SANGAREDDY, TELANGANA SANGAREDDY ----------- -----------
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(57) Abstract :
Artificial Intelligence based approach to Predict the factors responsible for contamination of food chain through uncertainty modelling is the proposed invention. The proposed invention focuses on predicting the factors responsible for causing contamination of food. The invention aims at utilizing the algorithm so uncertainty modelling for analyzing the contaminants that are present in the food.

No. of Pages : 13 No. of Claims : 6

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शासकीय जर्नल

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10)Dr.A.SASI KUMAR
11)AJAY DUREJA
12)Dr. SACHIN SABHARWAL
Name of Applicant : NA
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No. of Pages : 13 No. of Claims : 6

MoU/ Collaboration

To, **December 2022**

The principal,

NTVSs.G.T.P. Collage, Nandurbar

Applicant: *Kirankumar Madhav Nehete*

Subject: *Request to facilitate lab for Research work.*

Reference: *Provisional registration No. for Ph. D*

Guide Name: *Dr. Gaurav Ramesh Gupta (KBCNMU/11/PGR/CHEMISTRY/1518/2020).*

Respected Sir,

Most respectfully I would like to state that myself Kirankumar Madhav Nehete currently seeking for admission of Ph. D in Chemistry (PET-2021) under the guidance of Dr.Gaurav Ramesh Gupta. Currently I am working in a paints and coating industry and taken alignment from my current employer to take admission in Kavayitri Bahinabai Chaudhari North Maharashtra University in the faculty of Chemistry. With the same context I want to proceed a research work in your collage lab under the guidance of Dr. Ramesh Gupta.

I would like to request you to allow me to work in your lab on PhD project. I will pay all the legal fees and other expenses required as per request and follow the rules and regulations of your college and university. I would like to request to you to kindly do needful.

Sincerely,

K.m. Nehete

Kirankumar Madhav Nehete

Attachment:

1. Permission letter from respective authority of employer (Asian Paints)
2. MOU sign with employer for Ph. D related work.
3. University Provisional admission letter

==

asianpaints

Asian Paints Limited
Asian Paints House
6A, Shantinagar,
Santacruz (East),
Mumbai 400055
T: (022) 6218 1000
F: (022) 6218 1111
www.asianpaints.com

Ref. No.: 110891
Date: October 04, 2022

TO WHOMSOEVER IT MAY CONCERN

This is to certify that Mr. KIRANKUMAR NEHETE (Employee No. 110891) is in the employment of our Company since September 14, 2011 till date. Currently, Mr. KIRANKUMAR is working as ASSISTANT MANAGER - TECHNOLOGY at TURBHE, TURBHE.

This is to state on record that the company has no objection against Mr. Kirankumar Nehete pursuing the PhD program at Kavayitri Bahinabai Chaudhari North Maharashtra University, Jalgaon or against him being involved in any publications related to this PhD. In this regard, a suitable Non-Disclosure Agreement (NDA) has been signed between Mr. Kirankumar Nehete and the company in September 2022 and the same is enclosed with this letter.

For Asian Paints Limited

Abhishek Chopra
Associate General Manager - Human Resources

asianpaints

Asian Paints Limited

Asian Paints Limited
Plot No. C - 3B/1, TTC Industrial Area
MIDC Pawne, Thane - Belapur Road
Turbhe, Navi Mumbai - 400 703

Tel : (+9122) 6250 3434 / 3535
Fax: (+9122) 6250 3650
www.asianpaints.com

Non-Disclosure Agreement

THIS NON DISCLOSURE AGREEMENT (the "**Agreement**") is made and executed at Mumbai as on 1st day of September, 2022

BETWEEN

Asian Paints Limited, a company incorporated under the Indian Companies Act, 1913 and governed under the Companies Act 1956 and the Companies Act, 2013, having its registered office at 6A, Shantinagar, Santa Cruz (East), Mumbai -400 055 (hereinafter referred to as "**APL**", which expression shall unless it be repugnant to the context or meaning thereof, be deemed to mean and include its successors in business and assigns) of the One Part

AND

KIRANKUMAR NEHETE, 36 an Indian citizen, having Permanent Account Number: AICPN3645E and residing at 505 Sadguru Universal Set 17,Khanda Colony Panvel, 410206. having its registered office at, (hereinafter referred to as the "Company", which expression shall unless it be repugnant to the context or meaning thereof, be deemed to mean and include its successors in business and permitted assigns) of the Other Part.

WHEREAS;

A. APL has been inter alia carrying on the business of manufacturing, selling and distributing paints, varnishes, primers and the like as manufacturers, sellers and distributors throughout India.

B. APL is desirous of NDA for employee (Kirankumar) who is pursuing further education (PHD).

C. For the aforementioned purpose APL is desirous of engaging/evaluating some consultant/contractor who will provide the NDA for employee (Kirankumar) who is pursuing further education (PHD), (hereinafter for the sake of brevity referred to as "the Business Purpose").

D. In the process; APL would be required to share certain Confidential information and intellectual property of APL. information. There could be a possibility that in this engagement, APL may disclose APL's Proprietary as well. The said information and / or data received is

x. Implement controls to safeguard confidentiality and integrity of indirect data arising of personal data processing required to be retained by law;

xi. Not by any act or omission, cause APL or any authorized user to be in breach of any legal requirement of which APL has previously informed Company in writing

16. ENTIRE AGREEMENT:

This Agreement represents the entire agreement and understanding between the Parties with respect to its subject matter and supersedes any prior or contemporaneous discussions, representations, or agreements, whether written or oral, of the Parties regarding this subject matter.

17. SEVERABILITY:

If any provision of this Agreement or part thereof is rendered void, illegal or unenforceable in any respect under any law, the validity, legality and enforceability of the remaining provisions shall not in any way be affected or impaired thereby.

IN WITNESS WHEREOF, this Agreement is executed as of the date first above written.

ASIAN PAINTS LIMITED	**KiranKumar Nehete**
By: Rajeev Kumar Goel	**By:** K.m.Nehete
(Signature)	**(Signature)**

1990
'A' Grade
NAAC Re-Accredited
(4th Cycle)

KAVAYITRI BAHINABAI CHAUDHARI NORTH MAHARASHTRA UNIVERSITY, JALGAON

KBCNMU/11/Ph.D./**Chem.**/Online/2022 Date : 01-12-2022

To,

Mr. KIRANKUMAR MADHAV NEHETE

Subject:- Provisional admission to Ph.D. Course in the Subject of Chemistry under the faculty of Science and Technology

Dear Student,

With reference to the above subject, it is to inform you that, based on your qualification/exemption for the PET 2021 examination, and allotment of guide, you are provisionally registered for Ph.D. course from the date as mentioned below. Your Ph.D. registration will be confirmed on successful completion of Pre-Ph.D. course work and presentation of research outline before RRC within a stipulated period as per rules (Regarding the programme of conduct of the course work, you are requested to visit University's website **https://www.nmu.ac.in**). The particulars of your admission are as under:-

Sr. No.	Particulars	
1.	Name of Guide	**Dr. Gupta Gaurav Ramesh**
2.	Name of Co-guide	
3.	Place of Research Work	Laboratory / Research Center recognized by KBCNMU, Jalgaon
4.	Provisional date of Registration	Guide Allocation Meeting **14-10-2022**
5.	Registration No.	KBCNMU/11/Ph.D./**Chem./907/2022**
6.	Application No.	**PHD-2021-NVAEQ1 [Exemption]** .
7.	Fees Payment Details	Paid **Rs. 22750.00** on **12-12-2022 16:53:35**

Your attention is also invited to the following points regarding Ph.D. course admission :-

1. You will have to abide by the rules made by the University from time to time as per provision under Section 60 of the Maharashtra Public Universities Act, 2016 and the rules for the admission for Degree of Doctor of Philosophy (Ph.D.) as per the UGC (Minimum standards and procedure for awards of Ph.D. degree) Regulation 2009 and 2016 and revised Ph.D. rules from time to time.
2. You are requested to pay the following fees as prescribed by the University Authorities from time to time within one month from the date of issue of this letter. **The yearly fees will be charged every year from the date of registration.**

A) To be deposited in the University

Sr. No.	Head	First Year (Fee) Rs.		Subsequent Years Fee Rs.	
		For Science & Technology	Other than Science & Technology	For Science & Technology	Other than Science & Technology
1.	Provisional Registration Fees	1000/-	1000/-	0	0
2.	Admission Fees	1500/-	1500/-	0	0
3.	Tuition Fees	8000/-	8000/-	8000/-	8000/-
4.	Library Fee	1500/-	1500/-	1500/-	1500/-
5.	Course Work Fee	3000/-	3000/-	--	--
6.	Coursework Examination Fees	1500/-	1500/-	--	--

7.	University Development Fund	1000/-	1000/-	1000/-	1000/-
8.	Student Welfare Fund	200/-	200/-	200/-	200/-
9.	Student Aid Fund	100/-	100/-	100/-	100/-
10.*	**Laboratory Fee ***	**3000/-**	**0**	**3000/-**	**--**
11.	Computer and Internet Charges	1000/-	1000/-	1000/-	1000/-
12.	e-Suvidha	50/-	50/-	50/-	50/-
13.	Extra Curricular Activities	250/-	250/-	250/-	250/-
14.	Magazine Fee	60/-	60/-	60/-	60/-
15.	Identity Card Fee	100/-	100/-	--	--
16.	Gymkhana, Sports Activities	200/-	200/-	200/-	200/-
17.	Ashwamedha Fee	50/-	50/-	50/-	50/-
18.	Yuva Mahotsav Fee	50/-	50/-	50/-	50/-
19.	Group Insurance Charges	40/-	40/-	40/-	40/-
20.	Disaster Management	100/-	100/-	100/-	100/-
21.	Medical Fee	50/-	50/-	50/-	50/-
Total (without deposits)(A)		**22750/-**	**19750/-**	**15650/-**	**12650/-**

*** The fees from Second year onwards shall be deposited at concerned Research Center.**

B) To be deposited at the concerned approved Research Center					
22.	Library Deposit	3000/-	3000/-	0	0
23.	Laboratory Deposit	3000/-	0	0	0
Total (B)		**6000/-**	**3000/-**	**0**	**0**
Grant Total (A+B)		**28750/-**	**22750/-**	**15650/-**	**12650/-**

Note :

1. **Rs. 100/- will be charged as late fee per month if the fees are not paid within the prescribed time limit.**
2. **In case of revision of fee structure, the students will have to pay the revised fee accordingly.**
3. You are required to apply for eligiblity certificate to the Research Section of this University after receipt of confirmed registration letter within six months from the date of issue of confirmed registration letter. The eligiblity fee is Rs. 500/- and late fees of Rs. 1000/- will be charged if the candidate fails to apply for eligiblity certificate within six months after confirmed date of registration.
4. To obtain eligibility ceritifcate within one year from the date of issue of confirmed registration letter is mandatory. otherwise your admission is liable to be cancelled..
5. Foreign/NRI students will have to pay five time of the existing fees as mentioned in the above Table as mentioned in 2 & 3.
6. The duration of Ph.D. course registration shall be valid upto six years from the date of Provisional registration.
7. You will have to do your research (for Science, Pharamacy, Engineering & Technology) in the laboratory/Research Center of your guide recognized by Kavayitri Bahinabari Chaudhari North Maharashtra University, Jalgaon. If the laboratory/Research Center of your guide is not recognized, you have to work at another recognized laboratory/Research Center; however, in such case, you will have to take co-guide from that place. **You have to produce attendance certificate for working not less than 180 days with the concerned guide/co-guide with application of asking permission for submission of synopsis.**
8. It is must to publish at least one research paper in referred journal and make two paper presentations in Conferences/Seminars and produce evidence for the same in the form of acceptance letter or the reprint.
9. If the candidate wish to cancel his/her registration or if his/her admission is cancelled by the University then all fees payable to his account must be paid by the candidate.
10. You will have to pay late fee and/or fine as per the rules made by the University authorities from time to time.
11. You will have to produce original willingness letter received from guide at the time of document verification. If there is any discrepancy found in verification of original documents and documents attached with the application form (eg : Caste Ceriticate / Validity Ceritificate / Non-Creamy Layer which is applicable etc) your admission will liable to be cancelled.

Thanking you,

Yours faithfully,

sd/-

(V. V Talele)
Deputy Registrar
Research Section

---------- This is a computer generated document hence does not require any signature. ----------

RESEARCH COLLABORATION

This **RESEARCH COLLABORATION** is entered into, on this date 01/07/2021

BETWEEN

NTVS's G. T. Patil Arts, Commerce and Science College, Nandurbar-(425412) represented herein by Principal, Prof. V. S. Shrivastava (hereinafter, referred as **'First Party'**, include its successors – in-office, administrators and assigns).

AND

Dadasaheb Devidas Namdeo Bhole College, Bhusawal-425201 represented herein by Principal, Prof. Dr. R. P. Phalak (hereinafter, referred as **'Second Party'**, include its successors – in-office, administrators and assigns).

(First Party and Second Party are hereinafter jointly referred to as 'Parties' and individually as 'Party')

NOW THEREFORE, IN CONSIDERATION OF THE MUTUAL PROMISES SET FORTH IN THIS MoU, THE PARTIES HERETO AGREE AS FOLLOWS:

- **Project-Based Learning**: First Party shall design project-based activities especially for Science, Technology, Engineering and Mathematics (STEM) subjects for students of Second Party helping them excel in these subjects.
- **Training**: First Party shall design modules for training on recent technologies and share knowledge with teachers and students of Second Party.
- **Career Counseling**: First Party shall conduct exclusive sessions with students of Second Party on futuristic careers in the fields of Science & Engineering, Commerce & Management, Pharmacy, etc.
- **Student Connect**: Second Party shall share student details with First Party for one-to-one interaction and guidance on projects, models, skill development, career enhancement etc.
- **College Tour**: Get students of Second Party to experience a guided tour to campus, colleges, classrooms, laboratories, libraries, etc. of First Party.

- **Newsletters**: Students of Second Party shall have access to newsletters of First Party.
- **Events**: Students of Second Party will be regularly invited to be part of knowledge-based events and activities of First Party.
- **Resource Sharing**: Teachers and Students of Second Party will have access to online repositories of First Party for educational purpose.
- **Partner**: Parties may mention as Partner on their website.
- **Alumni Connect**: First Party shall help to connect Alumni of both Parties.
- **Validity**: This Collaboration shall be valid for 5 years from the July, 2021 and each party shall be at full liberty to terminate the collaboration with mutual consent.
- **Free of Cost**: The services herein are free of cost for education purpose.

For

Dadasaheb Devidas Namdeo Bhole College, Bhusawal-425201

Signature:

PRINCIPAL
Dadasaheb Devidas Namdev Bho
Mahavidyalaya,Bhusawal

Name: Prof. Dr. R. P. Phalak

Designation: Principal

Date:01/07/2021

Seal:

For

NTVS's G. T. Patil Arts, Commerce and Science College, Nandurbar-425412

(Prof. Dr. V. S. Shrivastava)
Principal

PRINCIPAL
G.T.Patil Arts,Commerce &
Science College
NANDURBAR - 425 412 (M.S.)

Signature:

Name: Prof. V. S. Shrivastava

Designation: Principal

Date: 01/07/2021

Seal:

P.N-425412

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Thermo-physical Investigations of oils, N-(2-aminoethyl)-oleamide and Resulting Gels using TGA-DSC

NARENDRA S. JOSHI[1,2], GOVINDA P. WAGHULDE[2] and GAURAV R. GUPTA[3*]**

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ABSTRACT

Edible vegetable oils were gelled by using N-(2-aminoethyl)-oleamide. Oils in their free state were subjected to differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) analysis. The gels of these oils were prepared by using N-(2-aminoethyl)-oleamide as gelator and similar thermal analysis of the gels was carried out. The thermal analysis data obtained was used to determine specific heat capacity at constant pressure (C_p). The values were compared with the reported values of heat capacities. It is observed that the thermal properties and transitions of oils and gels, specific heat capacity is helpful parameter to understand the fundamentals of gels and gelation strategies.

Keywords: Organo-gelator, Gelation, Heat capacity, Thermal analysis, TGA, DSC.

INTRODUCTION

The vegetable oils and fats are composed of different triacylglycerols (TAG), i.e., esters of fatty acids and glycerol. The chemical as well as physical properties of oils and fats are related to their fatty acid and triacylglycerol composition.[1] In many food products, crystallization and melting behavior of the oils are important properties for functionality. These thermal properties are important for identification of vegetable oils and can be used in quantitative and qualitative ways.[2-6] In confectionery, dairy and margarine industries, some of these vegetable fats like milk fat, hydrogenated fats, cocoa butter, etc. exhibits specific thermal behavior, relating to their useful properties in food formulations and their enormous use. It is necessary to know the physical properties, chemical composition and thermal behavior of the edible vegetable oils for a sufficient control of processes and for framing standard parameters for each desired use.[7] The specific heat capacity at constant pressure (C_p) can be considered as one of the important and useful physical properties. The information of the specific heat capacities of the oils is very useful to determine their behavior during different industrial processes.

EXPERIMENTAL

Materials

The oils viz., sesame oil, mustard oil, citriodora oil were purchased from local market. All the chemicals (extra pure) used for synthesis of gelator were purchased from Fisher Scientific.

Instrumentation

TGA-DSC analysis

The TGA-DSC analysis of the synthesized gelator was carried out at Central Instrumentation Facility, Shivaji University, Kolhapur and is reported in our previous communication.[8]

Synthesis of gelator and the gels

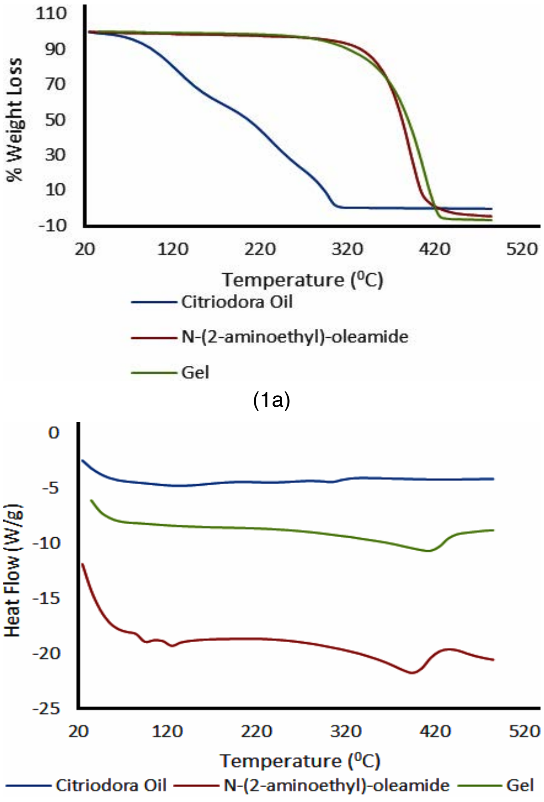
As reported in our earlier communication, several amide-based gelators were synthesized by using oleic acid as the precursor. Characterization of the synthesized gelator was done by using FTIR, ^{1}H-NMR, ^{13}C-NMR and Mass Spectral Analysis. A weighed quantity of the synthesized organo-gelators was added to the oil and the mixture was heated until all the gelator dissolves completely. The solution was then cooled to room temperature. Opaque gel forms slowly on cooling which was confirmed by inverting the tube.[8]

RESULTS AND DISCUSSION

Oils derived from wide variety of plants are an essential part of almost all the food products, and their structure related properties play a vital role in the production. The stat-of-the art exploration of these materials makes it essential to understand the complex structures and properties of these valuable materials. In addition to that, thermal analysis is the key tool in the arsenal of analytical chemistry for the elucidation of the structure related properties of these materials.[9-10]

Although, a systematic thermal analysis of variety of oils and food materials using TGA-DSC has already been reported very aptly in the literature and the results have been discussed very systematically.[11-14] However, adequate reports have not been found on the detailed thermal analysis of the gels of oils, in particular the specific heat capacity measurements of such gel using thermal methods. In the following pages, thermal profiles of citriodora oil, mustard oil, sesame oil and their corresponding gels with N-(2-aminoethyl)-oleamide have been discussed thoroughly.

Thermal analysis of Citriodora oil, N-(2-aminoethyl)-oleamide and gel



(1a)

(1b)

Fig. 1. TGA-DSC analysis of citriodora oil, N-(2-aminoethyl)-oleamide and gel

The closer scrutiny of the Fig. 1a, TGA of N-(2-aminoethyl)-oleamide and gel reveals a very sharp single stage decomposition over 300°C. The citriodora oil, a blend of triglycerides and free fatty acids, shows measurable pattern of decomposition as a function of temperature and possibly it is attributed to the composition and structural mesophasic changes occurred in such type of blends.[1] In Fig. 1b, the heat flow response and the formation of endothermic pattern for citriodora oil, N-(2-aminoethyl)-oleamide and their gel provides sound information about the smectic or mesophasic changes encountered in the oil and the gel. To our delight, it is to be observed that the resulting gel have transitory response between oil and gel.

Thermal analysis of Mustard oil, N-(2-aminoethyl)-oleamide and gel

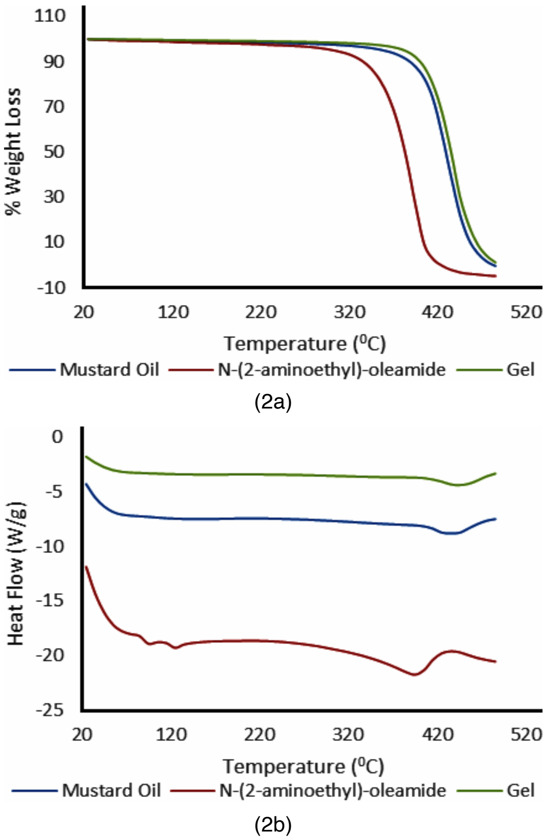


Fig. 2. TGA-DSC analysis of mustard oil, N-(2-aminoethyl)-oleamide and gel

The closer scrutiny of the Fig. 2a, TGA of mustard oil, N-(2-aminoethyl)-oleamide and gel reveals a very sharp single stage decomposition over 300°C. In Fig. 2b, the heat flow response and the formation of endothermic pattern for mustard oil, N-(2-aminoethyl)-oleamide and their gel provides sound information about the smectic or mesophasic changes encountered in the oil and the gel.

As mentioned earlier, all oils are blend of triglycerides and free fatty acids, and exhibited measurable pattern of decomposition as a function of temperature and possibly it is attributed to the composition and the structural mesophasic changes occurred in such type of blends.[1] It is to be noted that in case of mustard oil and its gel with N-(2-aminoethyl)-oleamide, interesting pattern of heat flow and endo-peaks have been observed in which the oil have a transitory response between gel and a gelator.

Thermal analysis of Sesame oil, N-(2-aminoethyl)-oleamide and gel

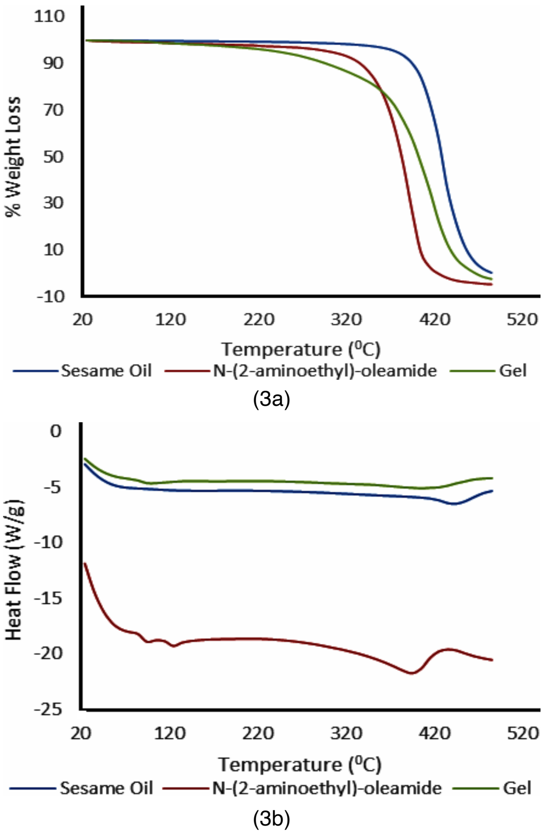


Fig. 3. TGA-DSC analysis of sesame oil, N-(2-aminoethyl)-oleamide and gel

The closer scrutiny of the Fig. 3a and 3b, TGA-DSC of sesame oil, N-(2-aminoethyl)-oleamide and gel reveals quite a similar pattern of decomposition as well as heat flow as a function of temperature with the previous mustard oil systems.

The utility of thermal methods towards the determination of thermal properties of oils or fats is one of the major areas of the application of thermal analysis (TGA-DSC). Till date, the thermal properties of quite a large number of oils and fats have extensively been studied using thermal methods like TGA and DSC. It is to note that the properties of oils and fats are intensely influenced by physio-chemical interactions, specifically among triglycerols (the fundamental species in oils and fats). The present literature also reveals that the physicochemical interactions present in the oils and the fats are very complicated, and a complete information and knowledge of their thermal properties requires a thorough examination of such interactions. As it is fact that we cannot have any first-hand information about the chemical composition of oils and fats based on these experiments. However, we can have a sound information about the science of the key thermodynamic changes that are associated with the phase transformation in the oil. Furthermore, these thermodynamic features are strongly depending on the general chemical composition of oils and fats and hence can be used for identification and full scope exploration of oils and fats, in qualitative and quantitative ways.

Thermal method (DSC) is particularly useful for studying the structure related interactions within the triglycerol components, because these techniques provide fundamental of the phase equilibrium diagrams for the studied systems, which provide a prowess of structure related information. It is also fact that beyond the compositional variation and their structure related interactions, the temperature-dependent polymorphic behavior of triglycerols in oils is responsible for their complicated thermal properties. On the other hand, DSC has advantage not only for thermodynamic analysis, but also for isothermal analysis of the system. Notably, the DSC profiles can also be explored towards the determination of one of the most important thermodynamic properties, i.e., specific heat capacity very systematically[15-17]. In the following pages, the specific heat capacity data for the studied systems are presented and discussed.

Specific heat capacity (C_p) of Citriodora oil, N-(2-aminoethyl)-oleamide and gel

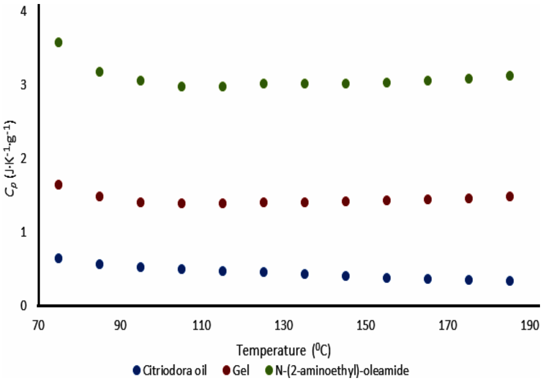


Fig. 4. Variation of specific heat capacity (C_p) of citriodora oil, N-(2-aminoethyl)-oleamide and gel as a function of temperature

From the Fig. 4, it is to be said that citriodora oil is the stable blend of triglycerols and have low specific heat capacity values than the corresponding gel.

Specific heat capacity (C_p) of Mustard oil, N-(2-aminoethyl)-oleamide and gel

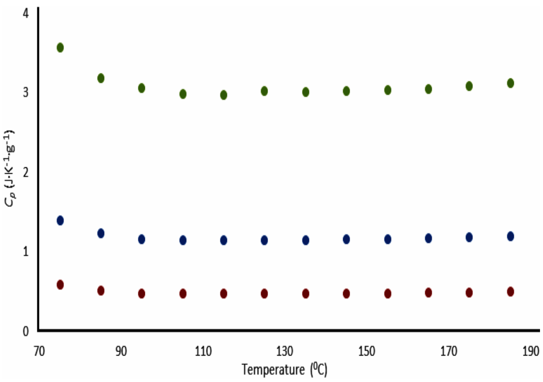


Fig. 5. Variation of specific heat capacity (C_p) of mustard oil, N-(2-aminoethyl)-oleamide and gel as a function of temperature

The closure scrutiny of Fig. 5 reveals that the gel of the mustard oil is quite stable as compared to the mustard oil.

Specific heat capacity (C_p) of Sesame oil, N-(2-aminoethyl)-oleamide and gel

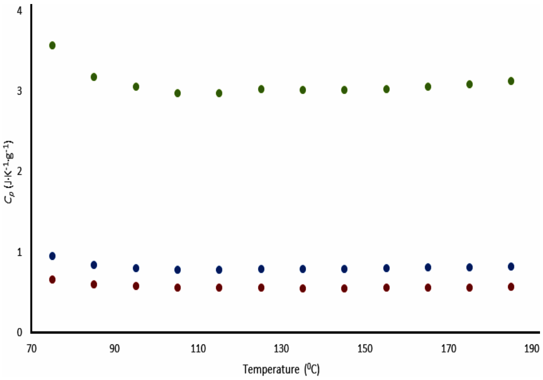
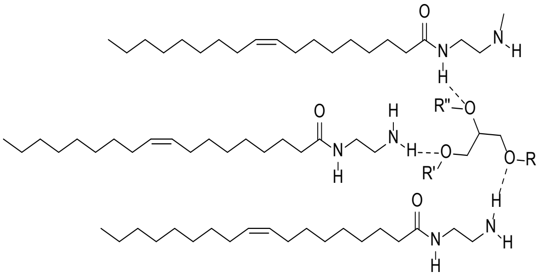


Fig. 6. Variation of specific heat capacity (C_p) of sesame oil, N-(2-aminoethyl)-oleamide and gel as a function of temperature

From the above Fig. 6, it is to be said that the gel of sesame oil is comparatively stable than the corresponding gel.

As we know, DSC is one of the widely used instrumental techniques for determination of the structure related properties of oils and other biomaterials, and it is to be applied very aptly in the field of oils and fats to understand wide variety of complex reactions viz., phase transitions, crystallization and melting processes, and lipid oxidation in the oils. Notably, all the structure related changes in oils and fats involve endothermic or exo¬thermic reactions. However, DSC is considered as a non¬specific analytical technique in order to measure the various structure related changes in oils and fats.

As specific heat capacity curves of the studied oils and their corresponding gels differ considerably, there is a basis for qualitative detection of adulteration or the presence of gelator from the perspectives of pure oils as noticed in the DSC curves (Fig. 1b, 2b, and 3b) as well as in specific heat capacity curves (Fig. 4–6). However, based on the characteristic composition, i.e., triglycerols of individual oils, the attempts have been made to comprehend the possible mechanism for the H-bonding interactions between oil and the gelator (Scheme 1).



Scheme 1: Possible H-bonding interactions between triglycerol part of the oil and N-(2-aminoethyl)-oleamide

CONCLUSION

The use of thermal analysis for understanding the gelation mechanism for the gel formation between oils and N-(2-aminoethyl)-oleamide on the basis of the chemical components is attempted here. The influence of triglycerols may find more information on further detailed investigation. Considering the huge global market in oils and gels, DSC could indeed be a useful technique for understanding thermal properties of oils and gels through characterization of the curves. In addition to that, new perspectives in the application of thermal methods to extract quality information about the studied systems are desirable. In the present study, it is found that the thermal properties and transitions of oils and gels, specific heat capacity is a benchmark parameter to understand the fundamentals of gels and gelation strategies. The DSC and thermal techniques are found to be very interesting for its application in food and related technology for academicians, researchers and industries in different sectors of food manufacture.

ACKNOWLEDGEMENT

We acknowledge the analytical services of CIF, Shivaji University, Kolhapur and the support from Dadasaheb Devidas Namdeo Bhole college, Bhusawal and Arts, Commerce and Science College, Bodwad for this work.

Conflict of Interest

The authors declare that we have no conflict of interest.

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Collaboration/Linkage Certificate

To whomsoever it may be concern

This is to certify that **Dr. Manohar RajendraPatil** Department of Chemistry **NTVS's G.T. Patil Arts, Commerce and Science College, Nandurbar-425412** has research collaboration (since 2020)with **P.R.High School Societie's Arts , Commerce and Science College, Dharangaon, Dist. Jalgaon-425105** for sharing the research ideas, exchange of reprints of our research papers and for the sample characterizations. We have jointly worked on research topics related to the application of nanoparticles and have published the research work in reputed international journals.

We have further extended this linkage with both the Chemistry departments to review the curriculum, teaching practices and discuss ways in which courses could be revised to promote scientific knowledge among the students.

Place: Dharangaon

(Prof. Dr. V. S. Shrivastava
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To,
Dr. Anil N. Kulkarni
Assistant Professor,
Department of Physics,
G.T. Patil ACS College,
Nandurbar- 425412.

Date 10/12/2020

Subject: Research Collaboration

Dear Anil,

I am writing this letter to express my support for your upcoming research work at Department of Physics, G.T. Patil ACS College, Nandurbar- 425412. At Advanced Physics Laboratory, SPPU, Pune, we work in the area of Materials science including synthesis, characterization and optoelectronic applications. Beyond this, our laboratory can provide a variety of characterization facilities such as Cyclic Voltammeter, Hall effect Measurement, Conductivity Measurement, Solar Cell JV Characteristics, UV-Visible Spectroscopy, Optical Microscopy and so on. Finally, our laboratory group would be delighted to help your group with any necessary advice or training required to implement your planned studies.

Best wishes for future endeavours.

Dr. Habib M. Pathan

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Chemical Solution Deposition of Sb_2Se_3 Films to Study their Structural, Morphological and Optical Properties

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Abstract

At room temperature chemical solution deposition technique has been employed for the deposition of Sb_2Se_3 thin films. Solution based deposition of Sb_2Se_3 crystals with variation in reaction time was found to be playing a significant role in controlling the reaction rate during the deposition of Sb_2Se_3 films. Temporal evolution of structural, morphological and optical properties of deposited Sb_2Se_3 films was investigated using X-ray diffraction (XRD), scanning electron microscopy and UV-visible spectroscopy, respectively. Solution deposition of Sb_2Se_3 films involves two steps: initial nucleation and crystal formation followed by growth to form final films. Increased reaction time from 30 to 120 min, deposited films showed morphological evolution for Sb_2Se_3 nanocrystals from dense spheres to self-assembled flower-like morphology. In addition, optical energy band gap variation from 1.60 to 1.63 eV suggested the possibility of crystal size optimization with energy band gap tunability of Sb_2Se_3 crystals in the visible region. This is also evident from the photoluminescence studies, which reveal the luminescence intensity variation with crystal size of Sb_2Se_3 as a function of deposition time. Optical and morphological response of Sb_2Se_3 crystals to the reaction conditions suggests it is a suitable and potential candidate for optoelectronic applications such as photovoltaic cells, electronic nano-devices, fuel cells, *etc*.

Keywords: Sb_2Se_3; Chemical solution deposition; XRD; Strain broadening; Photoluminescence.
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Article type: Research article.

1. Introduction

Recently, metal chalcogenides like CdS, PbS, PbSe, HgS, In_2S_3, In_2Se_3, Bi_2S_3, Bi_2Se_3, Bi_2Te_3, Sb_2S_3 and Sb_2Se_3, have attracted considerable attraction of researchers as promising materials in thermoelectric cooling and optical devices.[1-4] Among these materials, in recent time stibnite family members viz., Bi_2Se_3, Bi_2Te_3, Sb_2S_3 and Sb_2Se_3 have been immerged out as promising candidates.[5,6] This is possibly due to their alluring optical and electrical properties in the nano regime. However, in the case of stibnite family based chalcogenides, Sb_2Se_3 is expected to stand better in various applications like advanced energy conversion and storage (ECS) devices including fuel cells, photo-electrochemical water splitting cells, solar cells, Li-ion batteries and supercapacitors. This is because of higher absorption and broad spectral response of metal chalcogenides.[7-12]

Literature reveals that, the performance of these energy devices relies strongly on the properties of the nanostructured material. Such wide exposure to various applications of metal chalcogenides has been profited due to the employed variations in the synthesis methods materials resulting in the different crystal sizes and surface morphologies. In view of the above, development in the field of nanomaterial synthesis is believed to play a key role in future advances of the device grade applications.[13-16]

Therefore, to explore complete optical properties of Sb_2Se_3, it becomes very necessary to characterize the variation of the optical absorption including photoluminescence (PL) as function of deposition conditions. Numerous reports are available on the synthesis of nanocrystalline Sb_2Se_3.[17-20]

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However, countable communications deal with the chemical solution deposition of Sb2se3 followed by the studies on the optical properties including PL.[21,22]

Thus, in this work, Sb_2Se_3 nanocrystals have been synthesized using chemical solution deposition and an attempt has been made to explain the evolution of their morphology. Phase identification and structural analysis of the prepared samples were carried out systematically. Optical properties including photoluminescence studies of the prepared nanocrystals were conducted and the probable reasons for the resultant spectra were explained.

2. Experimental

In the present synthesis, solutions of $SbCl_3$ (0.01 M) and Na_2SeO_3 (0.01 M) were prepared in acetone and double distilled water, respectively in two different beakers, wherein $SbCl_3$ acts as a precursor of Sb^{3+} and Na_2SeO_3 that of Se^{2-}. The deposition process is discussed in the following steps. First, the bath for Sb^{3+} was prepared by adding 1 gm of $SbCl_3$ to 10 ml of acetone and stirred for 5 minutes until a uniform mixture was formed. Further, 10 ml of triethanolamine (TEA) (20%), a complexing agent was then prepared in double distilled water and added to the first bath containing antimony source to obtain Sb^{3+}-TEA complex. In the next event, a 2M Se^{2-} precursor solution was prepared in double distilled water under constant stirring of 10 minutes and slowly introduced into the Sb^{3+}-TEA complex precursor solution under constant stirring. TEA, a complexing agent helps for obtaining soluble species of Sb^{3+} in acidic medium during the reaction. The pH of the combined bath was adjusted to be around 8–10 by dropping 2-3 pellets of NaOH through vigorous stirring. Finally, previously cleaned glass slides were introduced into the beaker for further deposition. The colour of the mixture solution was observed to be changing from milky white to orange indicating the formation of Sb_2Se_3 species. Each sample was taken out after completing the desired reaction time of 30, 60 and 120 m, respectively. The samples deposited at room temperature were named as A, B and C, in the increasing order of reaction time of 30, 60 and 120 m, respectively.

The analysis of crystal structural, morphological and elemental properties of crystalline Sb_2Se_3 films were carried out using X-ray Diffractometry (XRD) (model: XRD, Rigaku "D/B max -2400", Cu K_α = 0.154 nm), Scanning Electron Microscope (SEM) (model: JEOL-JSM 6360-A) and energy-dispersive X-ray spectroscopy (EDX), respectively. A UV- Vis spectrophotometer (model: JASCO V-670) was used to record optical absorption spectra of crystalline Sb_2Se_3 films in the range of 200-800 nm at room temperature. The emission spectrum was obtained by using photoluminescence spectroscopy technique.

3. Results and discussions

3.1 The phase identification and structural analysis of Sb_2Se_3 films

Figure 1 shows the XRD patterns of samples A-C, respectively. XRD patterns for films show defined diffraction signatures around 21.50, 23.72, 27.13, 31.06, 34.42, 43.79, and 50.90º, indexed to (220), (101), (021), (221), (420), (440) and (351) hkl planes. The observed peaks were compared with the JCPDS card No. 72-1184, which confirms the orthorhombic phase for deposited Sb_2Se_3 crystals. The average crystallite size in each film sample was calculated using a standard method in the literature after incorporating due corrections for the strain induced broadening in the diffraction peaks.[23-24]

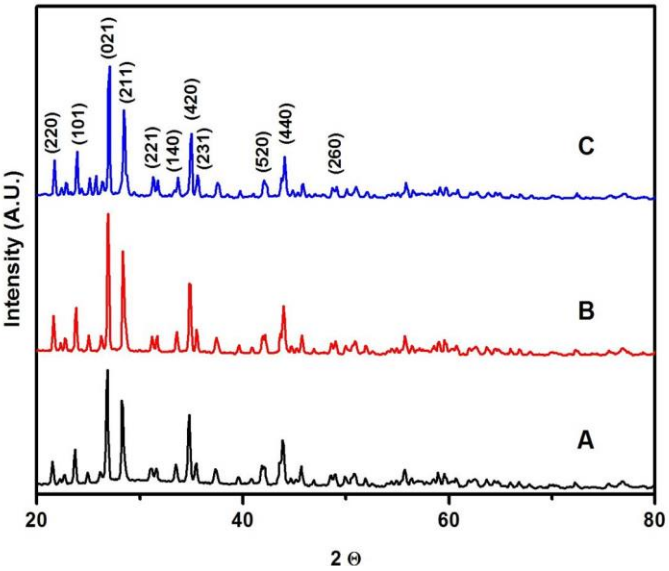

Fig. 1 Structural properties of Sb_2Se_3 films A, B and C.

Three main peaks of the obtained XRD pattern corresponding to (111), (230) and (221) planes were considered individually for each sample for the crystal size calculation. The average crystallite size was found to be in the range of 47-58 nm for the three samples considered. As known from the literature, the Equation 1,[16]

$$\beta \, \mathrm{Cos}\theta = \frac{K\lambda}{D} + n \, \mathrm{Sin}\theta \qquad (1)$$

where β is the full width at half maximum in radians of the diffraction peak under consideration after instrumental broadening correction, θ is the angle of diffraction, D is the size of the crystallite, ηis the strain in the material), and the plot about β Cosθ Vs η Sinθ is shown in Fig. 2. The Y-intercept of the plot corresponds to zero strain and so eliminates the strain induced line broadening. The average crystallite size D was then directly calculated from the Y-intercept ($=\frac{K\lambda}{D}$) for each sample. The results are tabulated in Table1.

In addition, to further prove the deposition of Sb_2Se_3 films, compositional analysis and elemental mapping were performed with the help of energy dispersive X-ray spectroscopy (EDXS) system as shown in Fig. 3. As illustrated in Fig. 2, composition mapping for Sb_2Se_3 films reveals the presence of Sb and Se in ~ 2:3 ratio, confirms the formation of Sb_2Se_3.

Table 1. Physical Parameters of all prepared samples.

Sample	2θ°	Sinθ	β_r(rad) × 10^{-3}	β_r COSθ × 10^{-3}	D (nm)
Film-A	21.50	0.1865	4.08	4.00	47
	23.72	0.2055	5.48	5.35	
	31.06	0.2677	6.7	6.45	
Film-B	21.50	0.1865	4.19	4.11	50
	23.72	0.2055	5.6	5.47	
	31.06	0.2677	6.82	6.56	
Film-C	21.50	0.1865	4.34	4.26	58
	23.72	0.2055	5.75	5.62	
	31.06	0.2677	6.97	6.71	

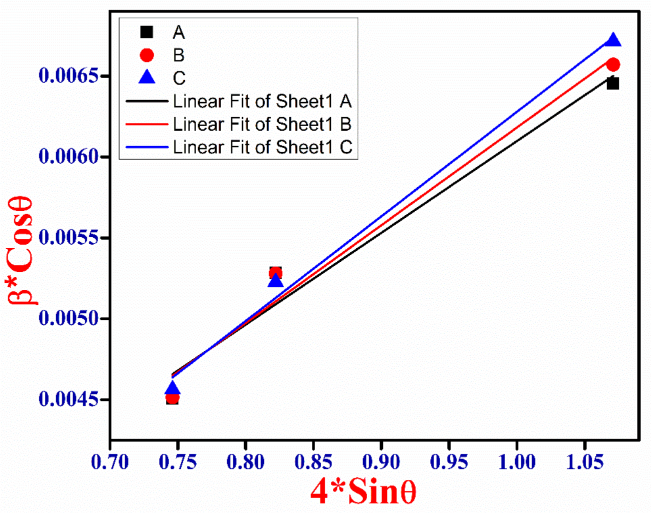

Fig. 2 Williamson-Hall plot for the estimation of crystallite size.

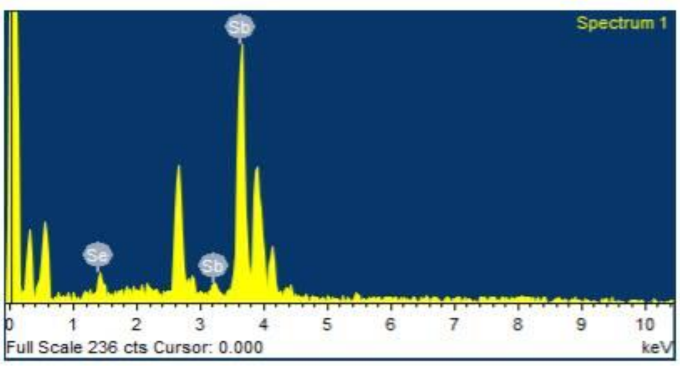

Fig. 3 Energy dispersive spectroscopic analysis of Sb_2Se_3 film A.

3.2 Morphological analysis of Sb_2Se_3 films

Figure 4 represents the SEM images for the samples A-C, respectively. At the initial stage of deposition *i.e.* for the first 30 minutes of reaction, the low magnification SEM image of sample A shown in (Fig. 4A$_1$) reveals the uniform and dense pinots-like morphology. However, higher magnification SEM images of sample A clearly represent the formation of self-assembled ring-like morphology for sample A (Fig. 4A$_2$). This may be due to the controlled nucleation of the Sb_2Se_3 species resulting into the observed morphology.

For the prolonged deposition time to 60 minutes *i.e.* sample B, the pinots are observed to be attached to rings (Fig. 4B$_1$). However, it is clearly seen from the higher magnification image (Fig. 4B$_2$) that, the pinots are getting interconnected and resulting into the thick petal-like morphology. Finally, for the deposition time of 120 minutes *i.e.* sample C, the temporal growth has resulted in the flower-like morphology (Figs. 4C$_1$ and C$_2$).

Observed morphological evolution in the present study, may be explained on the basis of the nucleation and growth kinetics of nanocrystals during the chemical solution deposition of the films. It appears that, reaction time has influenced the nucleation and growth of Sb_2Se_3 nanocrystals. During the initial deposition, reaction rate may have been driven by the Sb-TEA complex, which leads to control the release of Sb^{3+} in the reaction bath. As a result of this, in the initial phase of the deposition, the cationic and anionic species in the solution to be deposited get adsorbed over the embryo or nuclei and start growing into a crystal to give pinots like morphology. However, literature suggests that, during chemical solution deposition, the resultant morphology is the function of balance between surface and thermodynamic equilibrium. Thus, with prolonged deposition time early formed crystals start to self-organize in order to have minimum surface free energy. This is evident from the emergence of the different morphologies such as ring-like, petals and flower-like morphologies observed in the present study. This is in agreement with the numerous varieties of morphologies like nano-ribbons, nano-wires, hollow nano-spheres and solid nanospheres of Sb_2Se_3 reported in literature.[25-27]

3.4 Optical absorption Studies

Figure 5a shows the wavelength dependent absorption spectra of the samples A-C recorded in the range 350-850 nm. The UV-visible absorption spectra for samples A-C showed panchromatic absorbance behaviour with spectral response in the extended visible region. However, there is no significant difference in the absorption edge for samples from A to C, indicating no later variation in the crystallite size over

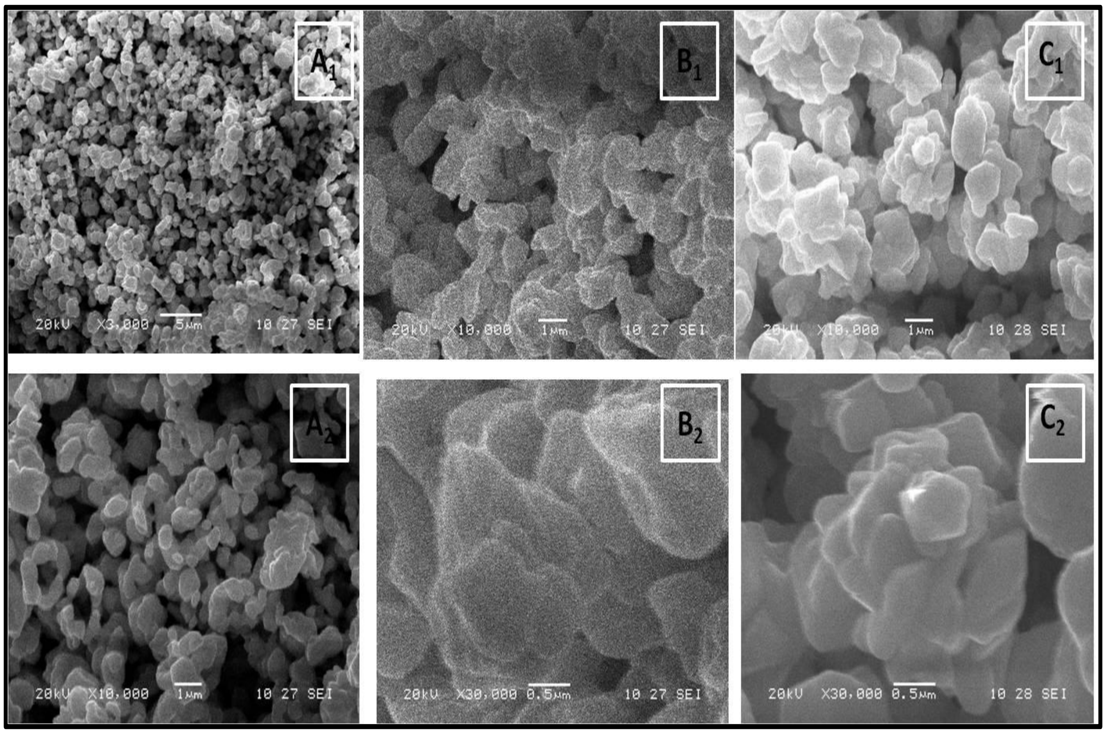

Fig. 4 Morphological analysis of films A, B and C.

prolonged reaction time, respectively. This is in agreement with the earlier discussion in XRD analysis. This is also in close with the optical results discussed in previous reports.

Figure 5b shows the optical band gap calculations for samples from A-C using optical absorption spectra using Equation 2.[19] Band gap plots depict the optical energy band gap (Eg) values in the range of 1.60 to 1.63 eV, respectively.[28] These values of Eg are quite greater than the bulk band gap value *i.e.* 1.2 eV of Sb_2Se_3 crystals, which can be attributed to the size reduction of the Sb_2Se_3 crystals during temporal deposition. This is in agreement with the earlier reports discussing the optical properties of metal chalcogenides.[29-31]

$$\alpha h\upsilon = \beta\,(h\upsilon - E_g)^n \tag{2}$$

3.5 Photoluminescence studies

Photoluminescence (PL) spectra of the samples A-C, recorded at room temperature with an excitation wavelength of 350 nm, has been presented in Fig. 6. The emission spectrum for all samples exhibits one distinct peak centred on 602 nm. The emission peaks in the present study for chemically deposited crystalline Sb_2Se_3 showed increase in intensity with the increase in reaction time.[1] This may be due to the prolonged reaction time resulting into the variation in morphology. According to literature, the morphological geometry controls the amount of scattering of light from the surfaces of the film. This may be evident from the variation into the PL intensities for different morphologies in the present work.[32,33] Thus, the observed enhancement of the PL emission can also be attributed to a low light scattering due to the reduction in the surface defects for Sb_2Se_3 crystals in the present study.[33]

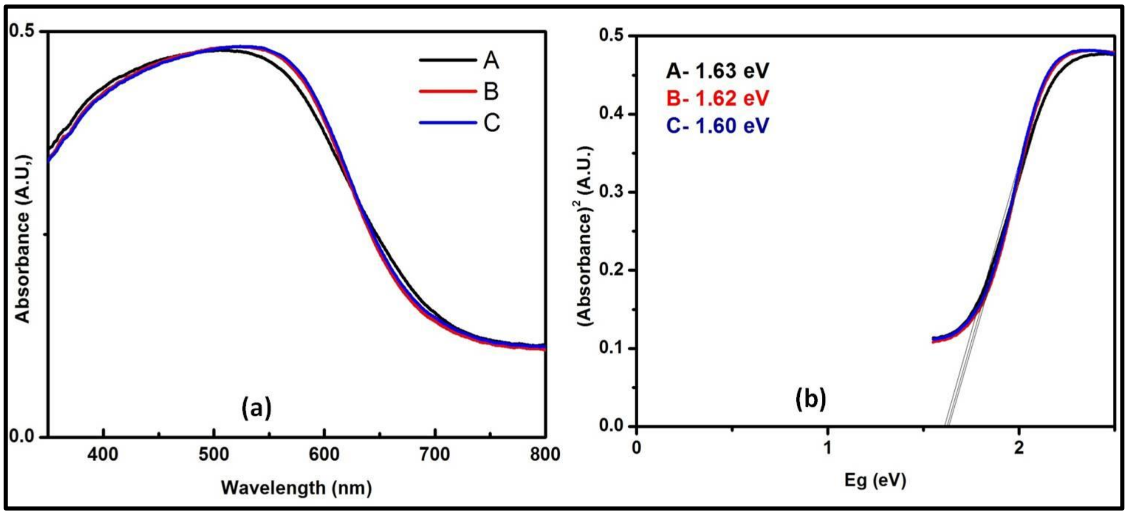

Fig. 5 Optical absorption spectra of films A, B and C.

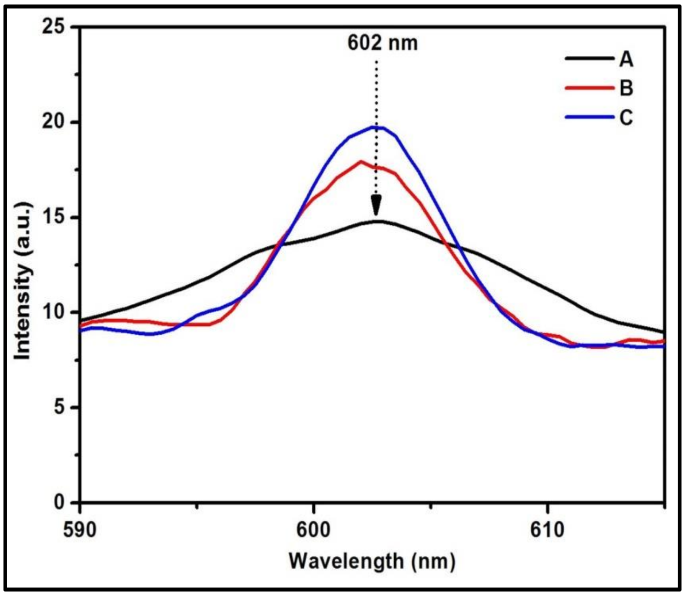

Fig. 6 Spectroscopy of films A, B and C.

3.6 Contact angle measurement

Measuring contact angles is a simple means to analyze wettability of thin film surfaces.[34] In the present study, in order to measure the contact angle, the water droplet was added on the copper surface by means of a syringe and the image of the drop was captured with a video camera. It was found that water droplets rest on the surface of Sb_2Se_3 films with a contact angle of about 60° revealing the hydrophilic nature of the deposited films (Fig. 7). This is in agreement with earlier report for different chemically deposited semiconducting material in the literature.[12] Such a hydrophilic nature of deposited Sb_2Se_3 finding applications in heterojunction based optical devices.

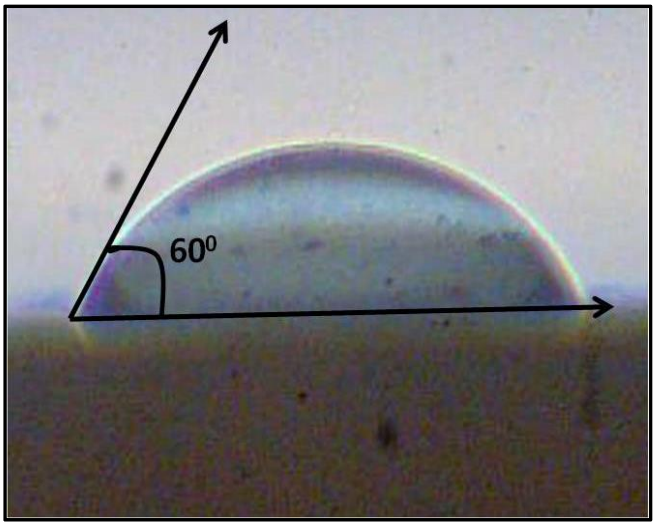

Fig. 7 Contact angle measurement of films A, B and C.

4. Conclusions

Role of the deposition time during the solution deposition of Sb_2Se_3 crystals through systematic experiments with its significance has been studied orderly. The deposition time was found to be playing an important role in the structural, morphological and optical properties of Sb_2Se_3 nanocrystals. The temporal growth of Sb_2Se_3 nanocrystals resulting into the variation in morphologies has been observed. This is been attributed to the super saturation factor and reaction rate during the deposition of crystals. Optical properties including PL found to be driven by size and shape of Sb_2Se_3 crystals. Observed morphological and optical properties reveal Sb_2Se_3 a promising absorber material in opto-electronic applications including photovoltaic devices.

Acknowledgement

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Conflict of Interest

There is no conflict of interest.

Supporting Information

Not applicable.

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We have further extended this linkage with both the Chemistry departments to review the curriculum, teaching practices and discuss ways in which courses could be revised to promote scientific knowledge among the students.

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Solvent-free grindstone synthesis of four new (*E*)-7-(arylidene)-indanones and their structural, spectroscopic and quantum chemical study: a comprehensive theoretical and experimental exploration

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ABSTRACT
In the present examination, four new compounds of (*E*)-7-(arylidene)-indanone skeleton have been synthesised using a grindstone chemistry approach; environmentally viable protocol. For a detailed molecular structure description, some quantum-chemical calculations of (*E*)-7-(arylidene)-indanones were performed by using the density functional theory method with a basis set B3LYP/6-311G(d,p). The optimised molecular geometry, quantum and structural entities such as bond length, bond angle, total energy, electron density distribution in highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), charge distribution, electronegativity, absolute hardness, softness, electrophilicity, chemical potential, charge transfer in molecules have been computed. All the compounds are well characterised using analytical methods; proton magnetic resonance (PMR) and carbon magnetic resonance (CMR) spectroscopy. Absorption energies, oscillator strength, and transitions of all four molecules have been calculated at TD-B3LYP/6-311G(d,p) level of theory for B3LYP/6-311G(d,p) optimised geometries. The molecular electrostatic surface potential plots have been computed for the better understanding of reactive sites. Some thermodynamic functions were also explored using theoretical calculations. All the calculations have been computed in the gas phase.

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DFT; B3LYP/6-311G (d,p); HOMO–LUMO; molecular electrostatic surface potential; grindstone synthesis

1. Introduction

The density functional theory based on theoretical quantum calculations has been effectively used in various fields of science [1–5]. Analysis of spectroscopic and quantum calculations is found to be very significant to envisage various quantum chemical parameters and thermodynamic aspects [6–10]. Some noteworthy examples of the application of Density functional theory (DFT) are equilibrium isotopic fractionation, cross-coupling reaction, pericyclic reaction, density-viscosity study, catalysis, and photoelectronic applications [11–16]. DFT calculations are dependable and significant for deciding the structure and various vital properties of molecules. Specifically, DFT calculations provide a good description of electronic and chemical bonding and give harmonic frequencies in the right agreement to experiment [17–19]. Quantum calculations based on DFT for FT-IR spectroscopy have stepped forward to the point where they could provide reliable vibrational spectra corresponding to the experiment [20–24]. Arylidene indanone scaffolds comprising of the characteristic indanone moiety with exocyclic double bond attached to an aryl/alkyl/heteroaryl group. Arylidene indanone scaffolds are found to exhibit an amazing profile of biological properties. Arylidene indanone motifs have been researched as inhibitors of monoamine oxidase [25], tubulin assembly inhibitors [26], acetylcholinesterase inhibitors in Alzheimer's disease treatment [27], and inhibitors of dual specificity phosphatase [28]. Importantly 2-arylidene indanone structures have also been investigated as inhibitors of leukemia [29], lung cancer [30], and breast cancer [31]. Additionally, they have been also found to be active as antimicrobial [32], antioxidant [33], anti-inflammatory [34], and antimalarial agents [35]. Donepezil is an outstanding medicine which contains indanone structure; used as an inhibitor of acetylcholinesterase in the Alzheimer's disease treatment. This medication improves neurocognitive function in patients suffering from Alzheimer's disease [36].

During the previous decade, there have been numerous green methodologies developed for the synthesis of a variety of organic compounds [37–47]. With the developing concern of environmental health by chemical waste, it becomes extremely appealing and important to imply green methods for the synthesis of organic compounds. With this viewpoint, the use of a solvent-free and grindstone chemistry approach for conducting organic synthesis is most vital in terms of green chemistry. Solvent-free processes are simple in terms of product isolation subsequently reducing waste production and ultimately cost also. In continuation of our previous work and by considering these vital aspects, a successful attempt has been made to apply a green strategy for the synthesis of arylidene indanone motifs and investigate structural parameters

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such as total energy, the electron density in highest occupied molecular orbital and lowest unoccupied molecular orbital, charge density, absolute electronegativity, softness, hardness and electron transferred of previously synthesised arylidene indanones. Additionally, the quantum-chemical calculations were used for a better understanding of the various properties as well as for an analysis of the geometrical parameters in the title molecule.

2. Experimental

2.1. Methods and materials

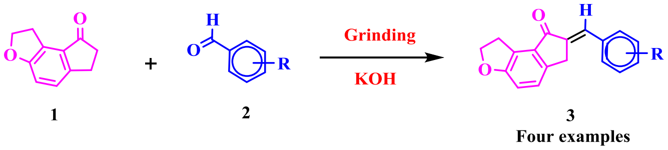
1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one was purchased from Henan Tianfu Chemical Co., Ltd., Zhengzhou, China, and other chemicals (Make: Merck, Sigma Aldrich, and Avra synthesis) with high purity were purchased from sigma laboratory, Nashik. The chemicals were used as received without any further purification. Melting points were determined in open capillary and uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker using $CDCl_3$ as a solvent. Reactions were monitored by thin-layer chromatography using aluminium sheets with silica gel 60 F254 (Merck).

2.1.1. Experimental procedure for the synthesis of (E)-7-arylidene-1,2,6,7-tetrahydro-8H-indeno[5,4-b]furan-8-ones

The room temperature solvent-free Claisen–Schmidt reaction of 1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one (**1**, 8 mmol) and aromatic aldehydes (**2**,10 mmol) in the presence of an equimolar quantity of solid KOH using mortar and pestle that resulted in the formation of corresponding (*E*)-7-arylidene-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-ones (Scheme 1). The reaction was monitored by using thin-layer chromatography (hexane-ethyl acetate; 7:3). The products were isolated by adding ice-cold water and purified by using hot ethanol.

2.1.2. Computational study

DFT calculations were performed using the Gaussian-03 program package without any constraint on the geometry [48]. The geometry of the molecules studied in this is optimised by DFT/B3LYP method using a 6-311G (d,p) basis set. The FMO analysis and quantum chemical study have performed using same basis set. Absorption energies (λ in nm), oscillator strength (f), and transitions of all four molecules have been calculated at TD-B3LYP/6-311G (d,p) level of theory for B3LYP/6-311G (d,p) optimised geometries. To investigate the reactive sites of the title molecules, the molecular electrostatic potential was computed using the same method. All the calculations were carried out for the optimised structure in the gas phase.



Scheme 1. (Colour online) Solvent-free synthesis of (*E*)-7-arylidene-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one at room temperature.

3. Results and discussion

3.1. Chemistry

As a model reaction when we performed solvent-free reaction of 1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one with 4-methyl benzaldehyde, we ended up in the formation of corresponding 7-arylidene indanone within 12 min. Inspired by this fantastic outcome, we carried out a similar reaction with other aromatic aldehydes and to our credit, all the reactions yielded desired products in excellent yield and that within twelve minutes (Table 1). The synthesised products have been successfully characterised by using ^{1}H NMR and ^{13}C NMR spectroscopic methods.

3.2. Physical and spectral data

(E)-7-(4-methylbenzylidene)-1,2,6,7-tetrahydro-8H-indeno[5,4-b]furan-8-one (3a): Yield: 95%; yellow solid; m.p. 108 °C;^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 2.40 (s, 3H), 3.55 (t, J = 8.8 Hz, 2H), 3.94 (d, J = 2.1 Hz, 2H), 4.67 (t, J = 8.9 Hz, 2H), 7.02 (d, J = 8.1 Hz, 1H), 7.31–7.22 (m, 3H), 7.59–7.52 (m, 3H);^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 28.54, 31.99, 72.51, 112.54, 116.15, 118.52, 125.06, 125.29, 130.78, 130.86, 132.57, 134.15, 138.91, 139.84, 141.22, 160.78, 194.04.

(E)-7-(2-methylbenzylidene)-1,2,6,7-tetrahydro-8H-indeno[5,4-b]furan-8-one (3b): Yield: 93%; yellow solid; m.p. 140°C;^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 2.49 (s, 3H), 3.58 (t, J = 8.9 Hz, 2H), 3.92 (d, J = 2.1 Hz, 2H), 4.70 (t, J = 8.9 Hz, 2H), 7.03 (d, J = 8.1 Hz, 1H), 7.30–7.25 (m, 4H), 7.65–7.61 (m, 1H), 7.87 (m, 1H);^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 20.14, 28.55, 31.70, 72.46, 115.54, 124.75, 125.17, 126.07, 128.62, 129.38, 130.82, 131.12, 134.21, 134.67, 136.48, 139.24, 141.95, 160.47, 194.64.

(E)-4-((8-oxo-1,2,6,8-tetrahydro-7H-indeno[5,4-b]furan-7-ylidene)methyl)benzonitrile (3c): Yield: 84%; yellow solid; m.p. 179 °C;^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 3.57 (t, J = 8.9 Hz, 2H), 4.02–3.98 (m, 2H), 4.71 (t, J = 8.9 Hz, 2H), 7.07 (d, J = 8.1 Hz, 1H), 7.32–7.27 (m, 1H), 7.56 (m, 1H), 7.74 (s, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 28.54, 31.99, 72.51, 76.78, 77.04, 77.29, 112.54, 116.15, 118.52, 125.06, 125.29, 130.78, 130.86, 132.57, 134.15, 138.91, 139.84, 141.22, 160.78, 194.04.

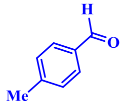
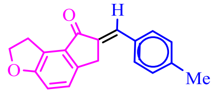
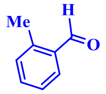
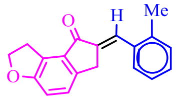
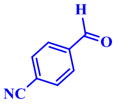
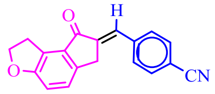
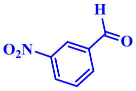
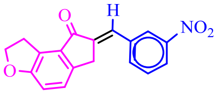
(E)-7-(3-nitrolbenzylidene)-1,2,6,7-tetrahydro-8H-indeno[5,4-b]furan-8-one(3d):

Yield: 90%; yellow solid; m.p. 146 °C;^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 3.58 (t, J = 8.4 Hz, 2H), 4.08–4.04 (m, 2H), 4.75–4.68 (m, 2H), 7.08 (m, 1H), 7.34 (m, 1H), 7.65 (m, 2H), 7.94 (d, J = 7.8 Hz, 1H), 8.25 (d, J = 8.4 Hz, 1H), 8.54 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm): 28.55, 31.86, 72.51, 116.17, 123.84, 124.33, 125.03, 125.38, 129.96, 130.34, 134.14, 136.47, 137.12, 138.46, 141.24, 148.66, 160.78, 194.03.

3.3. Computational study

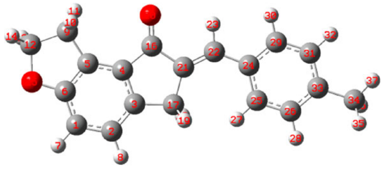
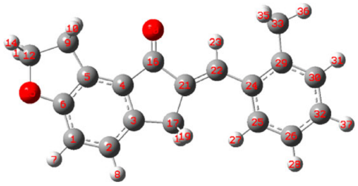
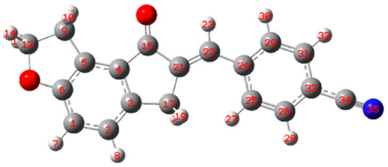
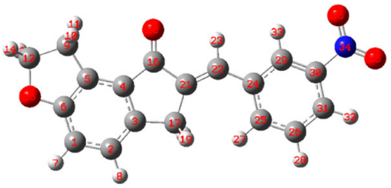
The structures of the four new 7-arylidene indanones (**3a**–**3d**) are presented in Table 2. The optimised molecular structures obtained by using the density functional theory method with

Table 1. Physicochemical data of (*E*)-7-arylidene-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one derivatives[a].

Entry	Aromatic aldehyde	Product	Time (min)	Yield[b] (%)	M.P. (°C)
3a			12	95	108
3b			10	93	140
3c			7	84	179
3d			5	90	146

[a] Reaction conditions: 1 (8 mmol), 2 (10 mmol).
[b] Yield of pure isolated product.

Table 2. Optimised molecular structures with IUPAC names and abbreviations.

Entry	IUPAC name of the products	Abbreviations	Optimised molecular structure
3a	(*E*)-7-(4-methylbenzylidene)-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one	**MBIF-1**	
3b	(*E*)-7-(2-methylbenzylidene)-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one	**MBIF-2**	
3c	(*E*)-4-((8-oxo-1,2,6,8-tetrahydro-7*H*-indeno[5,4-*b*]furan-7-ylidene)methyl)benzonitrile	**OIFB**	
3d	(*E*)-7-(3-nitrolbenzylidene)-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one	**NBIF**	

a basis set 6-311G (d,p). The point group symmetry for all four molecules is C1. The molecule **NBIF** has the highest polarity (μ = 5.7058 Debye) whereas the molecule **MBIF-2** has the lowest polarity (μ = 1.7983 Debye) amongst all four molecules. The large polarity difference is attributed to the presence of two substituents having an opposite electronic effect. In the molecule NBIF, the high dipole moment is a consequence of the captodative effect type of phenomenon. From one side electron donor group is attached and from other side electron acceptor group is attached. A similar effect is present in the molecule OIFB. The captodative phenomenon is presented in Figure 1.

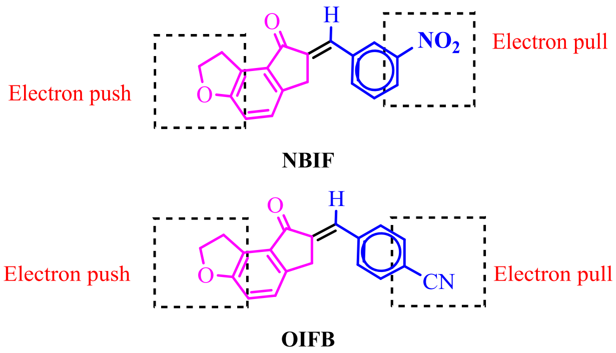


Figure 1. (Colour online) Captodative type phenomenon in NBIF and OIFB.

The optimized geometrical parameters; bond lengths and bond angles for all four molecules have been computed and presented here in Tables 3–6. In the molecule **MBIF-1**, the C4–C5 bond length is 1.386 Å which is the lowest amongst all C = C bond lengths. On the contrary, the highest bond length amongst all C = C bond lengths is C24–C25 bond length which is 1.408 Å. The carbonyl bond (C16–O20) has 1.219 Å distance while the alkene double bond (C21–H22) is 1.346 Å long. The longest and shortest aromatic C = C bonds in the molecule **MBIF-2** are C24–C29 (1.421 Å) and C25–C26 (1.388 Å) respectively. The carbonyl bond (C16–O20) has 1.219 Å bond length whereas the alkene double bond (C21–H22) length is 1.348 Å. In the case of the molecules **OIFB** and **NBIF**, the alkene C = C bond lengths are 1.345 and 1.344 Å respectively. In both the molecules, the longest aromatic C = C bond is C24–C25 whereas the shortest are C29–C31 (1.385 Å) and C4–C5 (1.389 Å) respectively. The CN bond is 1.155 Å long in the molecule **OIFB**. The C33–C34 bond in the molecule **OIFB** has acquired partial double bond character with 1.429 Å bond distance. This is due to the involvement of the CN group in resonance with the aromatic ring. The two NO bonds in the molecule **NBIF** (N34–O35 and N34–O36) are having nearly the same bond distance. The C = O bonds in **OIFB** and **NBIF** are 1.217 and 1.217 Å long respectively. All other bond lengths in all four molecules are also in good agreement. The C33–C34–N35 bond angle in the molecule **OIFB** is 179.93°. The O35–N34–O36 bond angle in the molecule **NBIF** is 124.97°. Remaining bond angle data is also found to be in good agreement.

Table 3. Optimised geometrical parameters of MBIF-1 at B3LYP/6-311 (d,p).

Bond lengths (Å)					
C1–C2	1.399	C9–C12	1.547	C25–C26	1.387
C1–C6	1.394	C12–H13	1.094	C25–H27	1.081
C1–H7	1.083	C12–H14	1.089	C26–H28	1.086
C2–C3	1.391	C12–O15	1.458	C26–C33	1.401
C2–H8	1.085	C16–O20	1.219	C29–H30	1.085
C3–C4	1.402	C16–C21	1.499	C29–C31	1.388
C3–C17	1.388	C17–H18	1.097	C31–H32	1.085
C4–C5	1.386	C17–H19	1.097	C31–C33	1.398
C4–C16	1.480	C17–C21	1.515	C33–C34	1.508
C5–C6	1.392	C21–H22	1.346	C34–H35	1.093
C5–C9	1.507	C22–H23	1.089	C34–H36	1.096
C6–O15	1.362	C22–C24	1.458	C34–H37	1.092
C9–H10	1.095	C24–C25	1.408	–	–
C9–H11	1.091	C24–C29	1.406	–	–
Bond angles (°)					
C2–C1–C6	118.64	C9–C12–H13	111.55	C25–C24–C29	117.19
C2–C1–H7	121.35	C9–C12–H14	114.04	C24–C25–C26	120.97
C6–C1–H7	120.00	C9–C12–O15	106.99	C24–C25–H27	120.26
C1–C2–C3	119.91	H13–C12–H14	109.13	C26–C25–H27	118.78
C1–C2–H8	119.38	H13–C12–O15	107.48	C25–C26–H28	119.20
C3–C2–H8	120.70	H14–C12–C15	107.34	C25–C26––C33	121.52
C2–C3–C4	120.25	C6–O15–C12	107.28	H28–C26–C33	119.28
C2–C3–C17	128.80	C4–C16–O20	126.84	C24–C29–H30	118.87
C4–C3–C17	110.95	C4–C16–C21	106.30	C24–C29–C31	121.56
C3–C4–C5	120.56	O20–C16–C21	126.85	C30–C29–C31	119.56
C3–C4–C16	110.06	C3–C17–H18	111.35	C29–C31–H32	119.48
C5–C4–C16	129.38	C3–C17–H19	111.35	C29–C31–C33	120.99
C4–C5–C6	118.31	C3–C17–C21	103.74	H32–C31–C33	119.53
C4–C5–C9	133.13	H18–C17–H19	106.80	C26–C33–C31	117.76
C6–C5–C9	108.50	H18–C17–C21	106.80	C26–C33–C34	120.86
C1–C6–C5	122.32	C19–C17–C21	111.86	C31–C33–C34	121.37
C1–C6–O15	124.38	C16–C21–C17	108.94	C33–C34–H35	111.37
C5–C6–O15	113.29	C16–C21–H22	119.41	C33–C34–H36	110.94
C5–C9–H10	110.63	C17–C21–H22	131.65	C33–C34–H37	111.44
C5–C9–H11	113.08	C21–C22–H23	113.63	C35–C34–H36	107.21
C5–C9–C12	101.10	C21–C22–C24	131.56	C35–C34–H37	108.13
H10–C9–H11	107.08	H23–C22–C24	114.81	C36–C34–H37	107.56
H10–C9–C12	112.29	C22–C24–C25	124.85	–	–
H11–C9–C12	112.72	C22–C24–C29	117.96	–	–

Table 4. Optimised geometrical parameters of MBIF-2 at B3LYP/6-311 (d,p).

Bond lengths (Å)					
C1–C2	1.399	C9–C12	1.547	C25–C26	1.388
C1–C6	1.394	C12–H13	1.094	C25–H27	1.080
C1–H7	1.083	C12–H14	1.089	C26–H28	1.084
C2–C3	1.391	C12–O15	1.458	C26–C33	1.392
C2–H8	1.085	C16–O20	1.219	C29–C30	1.396
C3–C4	1.402	C16–C21	1.501	C29–C33	1.512
C3––C17	1.518	C17–H18	1.097	C30–H31	1.085
C4––C5	1.388	C17–H19	1.096	C30–C32	1.392
C4–16	1.479	C17–C21	1.515	C32–H37	1.084
C5––C6	1.392	C21–H22	1.348	C33–H34	1.094
C5––C9	1.507	C22–H23	1.086	C33–H35	1.094
C6––O15	1.362	C22–C24	1.460	C33–H36	1.091
C9–H10	1.095	C24–C25	1.408	–	–
C9–H11	1.091	C24–C29	1.421	–	–
Bond angles (°)					
C2–C1–C6	118.64	H11–C9–C12	112.71	C22–C24–C25	122.45
C2–C1–H7	121.34	C9–C12–H13	111.55	C22–C24–C29	119.20
C6–C1–H7	120.02	C9–C12–H14	114.05	C25–C24–C29	118.35
C1–C2–C3	119.92	C9–C12–O15	106.97	C24–C25–C26	121.74
C1–C2–H8	119.38	H13–C12–H14	109.13	C24–C25–H27	119.58
C3–C2–H8	120.70	H13–C12–O15	107.49	C26–C25–H27	118.67
C2–C3–C4	120.24	H14–C12–O15	107.34	C25–C26–H28	119.92
C2–C3–C17	128.79	C6–O15–C12	107.27	C25–C26––C32	119.65
C4–C3–C17	110.97	C4–C16–O20	126.83	H28–C26–C32	120.43
C3–C4–C5	120.57	C4–C16–C21	106.39	C24–C29–C30	118.90
C3–C4–C16	110.04	O20–C16–C21	126.78	C24–C29–C33	122.18
C5–C4–C16	129.38	C3–C17–H18	110.96	C30–C29–C33	118.92
C4–C5–C6	118.30	C3–C17–H19	111.72	C29–C30–C31	118.82
C4–C5–C9	133.15	C3–C17–C21	103.79	C29–C30–C32	121.82
C6–C5–C9	108.49	H18–C17–H19	106.77	H31–C30–C32	119.36
C1–C6–C5	122.31	H18–C17–C21	111.79	C26–C32–C30	119.54
C1–C6–O15	124.39	C19–C17–C21	111.91	C26–C32–H37	120.45
C5–C6–O15	113.30	C16–C21–C17	108.80	C30–C32–H37	120.01
C5–C9–H10	110.64	C16–C21–H22	118.82	C29–C33–H34	111.91
C5–C9–H11	113.10	C17–C21–H22	132.37	C29–C33–H35	111.94
C5–C9–C12	101.10	C21–C22–H23	112.46	C29–C33–H36	110.33
H10–C9–H11	107.09	C21–C22–C24	131.72	H34–C33–H35	107.11
H10–C9–C12	112.27	H23–C22–C24	115.81	H34–C33–H36	107.62
–	–	–	–	C35–C33–H36	107.71

The chemical reactivity of a molecule is administered by the charge density of HOMO and LUMO energy surfaces. The HOMO is known as an orbital that could go about as an electron contributor since it is the peripheral orbital containing electrons. The general structure with of 7-arylidene indanone with ring labelling is given in Figure 2. The pictorial illustration of the frontier molecular orbitals is given in Figure 3. The

Table 5. Optimised geometrical parameters of OIFB at B3LYP/6-311 (d,p).

Bond lengths (Å)					
C1–C2	1.399	C9–H11	1.091	C24–C25	1.409
C1–C6	1.395	C9–C12	1.547	C24–C29	1.409
C1–H7	1.083	C12–H13	1.094	C25–C26	1.385
C2–C3	1.391	C12–H14	1.089	C25–H27	1.080
C2–H8	1.085	C12–O15	1.458	C26–H28	1.083
C3–C4	1.403	C16–O20	1.217	C26–C33	1.403
C3-–C17	1.518	C16–C21	1.506	C29–H30	1.084
C4-–C5	1.389	C17–H18	1.096	C29–C31	1.385
C4–16	1.477	C17–H19	1.096	C31–H32	1.083
C5-–C6	1.392	C17–C21	1.514	C31–C33	1.402
C5-–C9	1.507	C21–C22	1.345	C33–C34	1.429
C6-–O15	1.361	C22–H23	1.089	C34–N35	1.155
C9–H10	1.095	C22–C24	1.459	–	–
Bond angles (°)					
C2–C1–C6	118.71	H10–C9–C12	112.68	C21–C22–C24	131.26
C2–C1–H7	121.32	H11–C9–C12	112.27	H23–C22–C24	114.91
C6–C1–H7	119.97	C9–C12–H13	111.63	C22–C24–C25	124.57
C1–C2–C3	119.86	C9–C12–H14	114.01	C22–C24–C29	117.73
C1–C2–H8	119.86	C9–C12–O15	106.97	C25–C24–C29	117.70
C3–C2–H8	120.73	H13–C12–H14	109.15	C24–C25–C26	121.10
C2–C3–C4	120.27	H13–C12–O15	107.44	C24–C25–H27	120.34
C2–C3–C17	128.65	H14–C12–O15	107.32	C26–C25–H27	118.56
C4–C3–C17	111.07	C6–O15–C12	107.37	C25–C26–H28	120.24
C3–C4–C5	120.59	C4–C16–O20	127.34	C25–C26-–C33	120.31
C3–C4–C16	110.07	C4–C16–C21	106.29	H28–C26–C33	119.45
C5–C4–C16	129.34	O20–C16–C21	126.37	C24–C29–H30	120.52
C4–C5–C6	118.25	C3–C17–H18	111.39	C24–C29–C31	121.68
C4–C5–C9	133.18	C3–C17–H19	111.36	C30–C29–H31	119.39
C6–C5–C9	108.52	C3–C17–C21	103.73	C29–C31–C32	120.52
C1–C6–C5	122.31	H18–C17–H19	106.89	C29–C31–C33	119.78
C1–C6–O15	124.35	H18–C17–C21	111.77	H32–C31–C33	119.70
C5–C6–O15	113.34	C19–C17–C21	111.78	C26–C33–C31	119.44
C5–C9–H10	110.64	C16–C21–C17	108.84	C36–C33–C34	120.22
C5–C9–H11	113.08	C16–C21–H22	119.13	C31–C33–C34	120.35
C5–C9–C12	101.14	C17–C21–H22	132.03	C33–C34–N35	179.93
H10–C9–H11	107.09	C21–C22–H23	113.83	–	–

HOMO and LUMO energies are very essential as they relate to ionisation enthalpy and electron affinity respectively. As shown by these two parameters, the compound reactivity changes with the structural framework. The examination of the wave function shows that the electron absorption corresponds to the excitation from the ground state to the first excited state.

The HOMO is seen to be chiefly at ring A and on the contrary; LUMO is distributed over the enone framework and ring B in all four molecules. Due to the presence of the nitro group in the **NBIF** molecule, the LUMO is significantly situated at ring B. The **NBIF** molecule has the lowest HOMO–LUMO energy gap (3.403 eV) amongst all molecules. This is due to the captodative phenomenon present in the molecule. The lower HOMO–LUMO energy gap demonstrates the inevitable charge transfer interactions taking place within the molecule. This is attributed to the presence of the both acceptor and donor groups the **NBIF** molecule. Similar effect is present in the **OBIF** molecule; however, the effect is less powerful. The molecules **MBIF-1** and **MBIF-2** have electron releasing groups at the opposite sides which augments the energy gap and therefore both molecules would possess less chemical reactivity in terms of an electron transfer. The HOMO reactivity ($E_{HOMO} = -5.988$) is the highest in the **MBIF-1** molecule while the LUMO reactivity ($E_{LUMO} = -2.852$) is the highest in the molecule **OIFB**. The reason for this is the presence of two electron releasing groups (OR and Me) in the **MBIF-1** molecule and one electron releasing (OR) and one electron withdrawing group (CN) in the **OIFB** molecule.

Table 6. Optimised geometrical parameters of NBIF at B3LYP/6-311 (d,p).

Bond lengths (Å)					
C1–C2	1.399	C9–H11	1.091	C24–C25	1.409
C1–C6	1.395	C9–C12	1.547	C24–C29	1.405
C1–H7	1.083	C12–H13	1.094	C25–C26	1.391
C2–C3	1.391	C12–H14	1.089	C25–H27	1.080
C2–H8	1.085	C12–O15	1.459	C26–H28	1.083
C3–C4	1.402	C16–O20	1.217	C26–C31	1.391
C3-–C17	1.518	C16–C21	1.506	C29–H30	1.385
C4-–C5	1.389	C17–H18	1.097	C29–C33	1.081
C4–16	1.478	C17–H19	1.097	C30–C31	1.390
C5-–C6	1.392	C17–C21	1.514	C30–N34	1.483
C5-–C9	1.507	C21–C22	1.344	C31–C32	1.081
C6-–O15	1.361	C22–H23	1.089	N34–O35	1.223
C9–H10	1.095	C22–C24	1.461	N34–O36	1.222
Bond angles (°)					
C2–C1–C6	118.68	H11–C9–C12	112.70	C22–C24–C25	124.76
C2–C1–H7	121.33	C9–C12–H13	111.65	C22–C24–C29	117.50
C6–C1–H7	119.99	C9–C12–H14	114.01	C25–C24–C29	117.74
C1–C2–C3	119.88	C9–C12–O15	106.96	C24–C25–C26	121.23
C1–C2–H8	119.40	H13–C12–H14	109.15	C24–C25–H27	120.04
C3–C2–H8	120.72	H13–C12–O15	107.44	C26–C25–H27	118.72
C2–C3–C4	120.29	H14–C12–O15	107.32	C25–C26–H28	119.72
C2–C3–C17	128.63	C6–O15–C12	107.36	C25–C26-–C31	120.73
C4–C3–C17	111.07	C4–C16–O20	127.30	H28–C26–C31	119.55
C3–C4–C5	120.57	C4–C16–C21	106.28	C24–C29–C30	119.98
C3–C4–C16	110.08	O20–C16–C21	126.41	C24–C29–H33	120.87
C5–C4–C16	129.35	C3–C17–H18	111.38	C30–C29–H33	119.14
C4–C5–C6	118.26	C3–C17–H19	111.33	C29–C30–C31	122.37
C4–C5–C9	133.18	C3–C17–C21	103.72	C29–C30–C34	118.78
C6–C5–C9	108.50	H18–C17–H19	106.93	H31–C30–C34	118.85
C1–C6–C5	122.31	H18–C17–C21	111.77	C26–C30–C30	117.94
C1–C6–O15	124.35	H19–C17–C21	111.80	C26–C31–H32	122.33
C5–C6–O15	113.33	C16–C21–C17	108.84	C30–C31–H32	119.73
C5–C9–H10	110.63	C16–C21–H22	119.09	C30–N34–O35	117.41
C5–C9–H11	113.09	C17–C21–H22	132.07	C30–N34–O36	117.62
C5–C9–C12	101.14	C21–C22–H23	113.94	O35–N34–O36	124.97
H10–C9–H11	107.08	C21–C22–C24	131.23	–	–
H10–C9–C12	112.25	H23–C22–C24	114.83	–	–

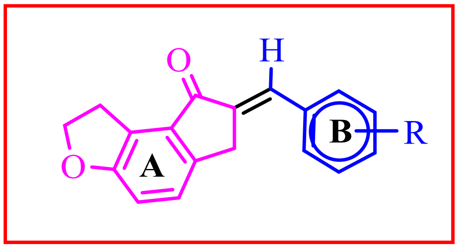


Figure 2. (Colour online) General structure with ring labelling.

The electronic parameters of all four derivatives are tabulated in Table 7. From the HOMO–LUMO information, it is affirmed that the presence of electron releasing group on ring A and electron attracting group on ring D results in lowering of the energy gap. On the contrary, the presence of an electron releasing group on ring B augments the energy gap. The quantum chemical parameters are presented in Table 8 and have been calculated from molecular parameters using Koopmans' theorem. The parameters like electronegativity (χ), absolute hardness (η), global softness (σ), global electrophilicity index (ω), chemical potential (Pi) maximum number of electron transferred (ΔNmax) have been established. All these parameters provide valuable insights into the chemical reactivity of molecules. The highest value of the electronegativity (χ = 4.557 **eV**) in the molecule **OIFB** suggests that it has the most powerful electron attracting property. The data of absolute

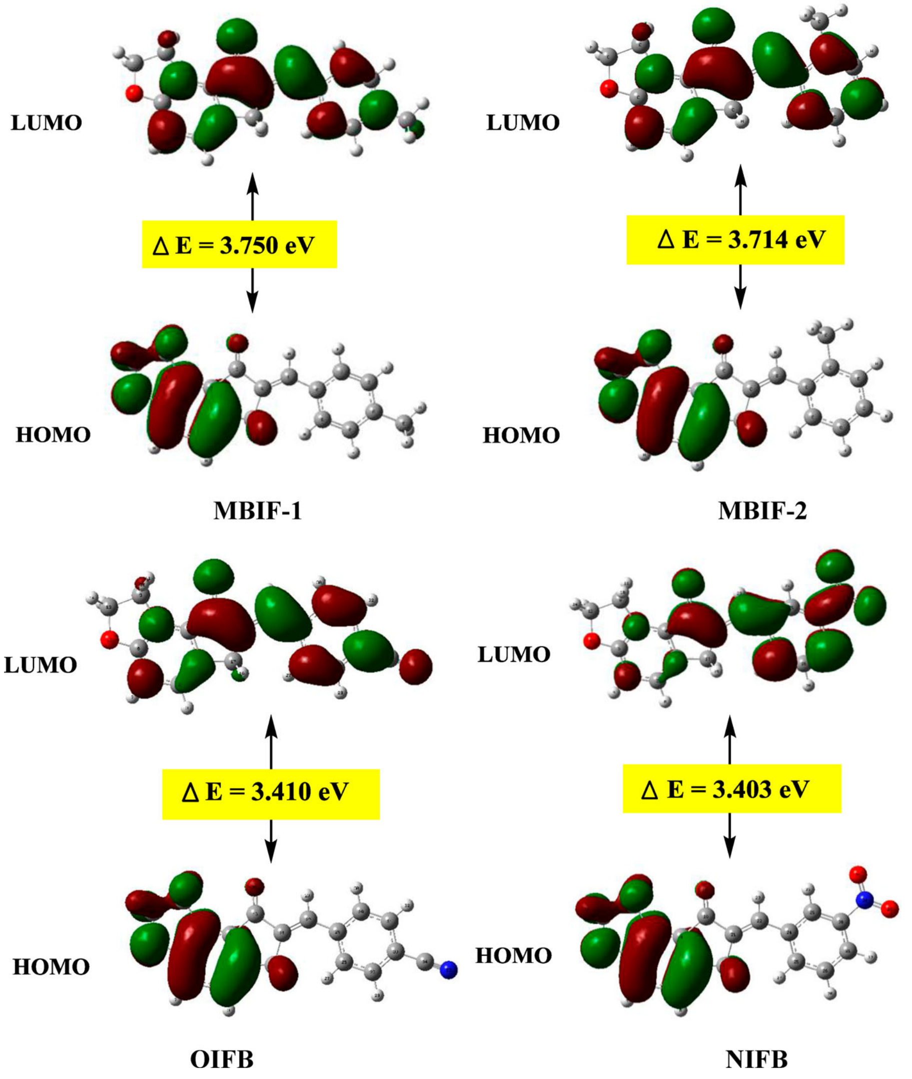


Figure 3. (Colour online) HOMO–LUMO pictures.

Table 7. Electronic parameters.

Name	E (a.u.)	E_{HOMO} (eV)	E_{LUMO} (eV)	I (eV)	A (eV)	Eg (eV)
MBIF-1	−884.323	−5.988	−2.237	5.988	2.237	3.750
MBIF-2	−884.320	−6.017	−2.303	6.017	2.303	3.714
OIFB	−1049.549	−6.262	−2.852	6.262	2.852	3.410
NBIF	−958.887	−6.252	−2.849	6.252	2.849	3.403

Note: Abbreviations: I, ionisation potential; A, electron affinity; Note: $I = -E_{HOMO}$ & $A = -E_{LUMO}$.

hardness and the global softness affirms that the molecule **MBIF-1** ($\eta = 1.875$ eV) is softer and the molecule **NBIF** ($\sigma = 0.588$) is harder in comparison with each other. This data is very crucial to decide the chemical reactivity. All the four molecules would undergo fast nucleophilic attacks; however, the molecule **NBIF** would prefer faster nucleophilic attacks as it has the highest value of global electrophilicity index ($\omega = 6.101$). The maximum charge transfer is taking place within the **OIFB** molecule due to high value of maximum number of electron transfer (ΔNmax = 2.6727 eV). By employing TD-B3LYP/6-311G (d,p) level of theory for B3LYP/6-311G (d,p) optimised geometries, absorption energies (λ in nm), oscillator strength (f), and transitions of all four molecules have been computed and depicted in Table 9. The S_0 to S_1 excitation energy data suggests that shifting from electron releasing to electron attracting group on ring B results in redshift. However, a molecule with a strong electron attracting nitro group has

Table 8. Global reactivity parameters.

Name	χ (eV)	η (eV)	σ (eV^{-1})	ω (eV)	Pi (eV)	ΔNmax (eV)	Dipole Moment (Debye)
MBIF-1	3.553	1.875	0.533	3.366	−3.553	1.8949	2.742
MBIF-2	4.160	1.857	0.538	4.660	−4.160	2.2404	1.798
OIFB	4.557	1.705	0.586	6.090	−4.557	2.6727	4.325
NBIF	4.551	1.702	0.588	6.101	−4.551	2.2738	5.706

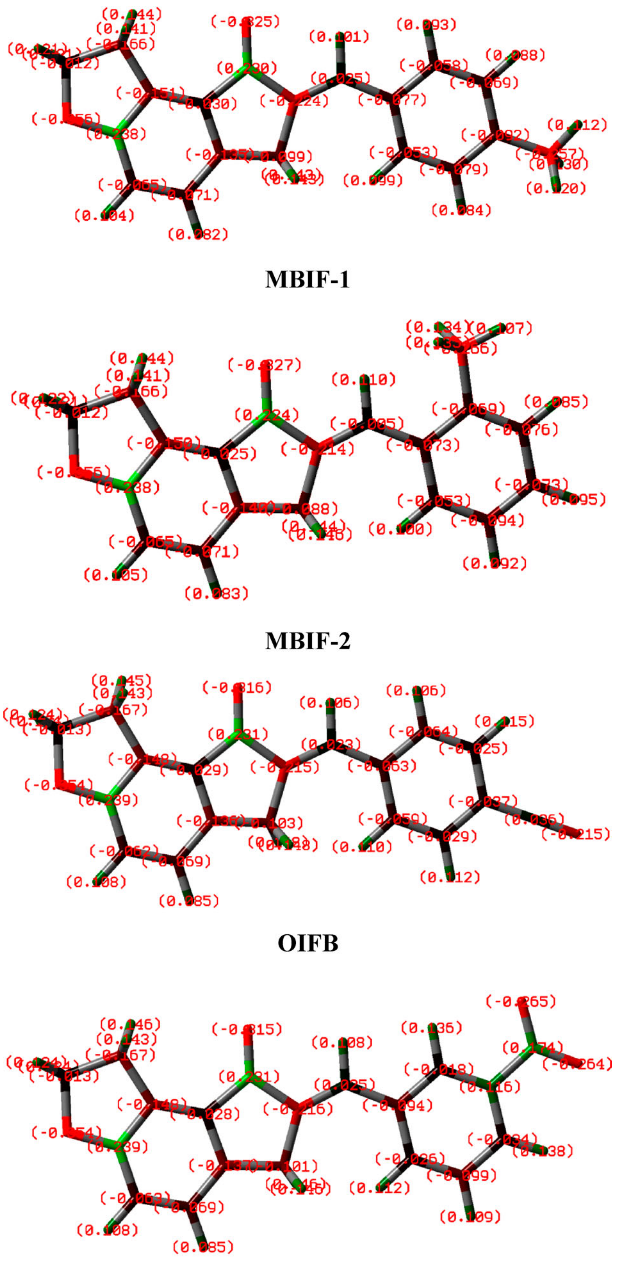
Note: $\chi = (I + A)/2$; $\eta = (I - A)/2$; $\sigma = 1/\eta$; $\omega = Pi^2/2\eta$; $Pi = -\chi$; $\Delta Nmax = -Pi/\eta$. Abbreviations: χ, electronegativity; η, absolute hardness; σ, global softness; ω, global electrophilicity; Pi, chemical potential; ΔNmax, maximum no. of electron transferred.

Table 9. Absorption energies (λ in nm), Oscillator strength (*f*), and Transitions of all four molecules computed at TD-B3LYP/6-311G (d,p) level of theory for B3LYP/6-311G(d,p) optimised geometries.

Name	State	λ^{abs}	*f*	Configuration	Transition
MBIF-1	S_0–>S_1	386.52	0.0116	73–>74	H–>L
MBIF-2	S_0–>S_1	390.94	0.0170	73–>74	H–>L
OIFB	S_0–>S_1	428.04	0.0120	75–>76	H–>L
NBIF	S_0–>S_1	420.47	0.0103	80–>81	H–>L

Table 10. Mulliken atomic charges of MBIF-1 and MBIF-2 molecules computed for B3LYP/6-311G (d,p) optimised geometries.

MBIF-1				MBIF-2			
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
1 C	−0.065	**20 O**	**−0.327**	1 C	−0.065	**20 O**	**−0.326**
2 C	−0.071	21 C	−0.222	2 C	−0.071	21 C	−0.211
3 C	−0.135	22 C	0.027	3 C	−0.141	22 C	−0.015
4 C	−0.030	23 H	0.101	4 C	−0.025	23 H	0.114
5 C	−0.152	24 C	−0.073	5 C	−0.151	24 C	−0.049
6 C	0.238	25 C	−0.057	6 C	0.238	25 C	−0.055
7 H	0.104	26 C	−0.075	7 H	0.105	26 C	−0.098
8 H	0.082	27 H	0.099	8 H	0.083	27 H	0.098
9 C	−0.166	28 H	0.086	9 C	−0.166	28 H	0.091
10 H	0.140	29 C	−0.061	10 H	0.141	29 C	−0.086
11 H	0.144	30 H	0.092	11 H	0.144	30 C	−0.073
12 C	−0.012	31 C	−0.065	12 C	−0.012	31 H	0.085
13 H	0.121	32 H	0.089	13 H	0.121	32 C	−0.070
14 H	0.121	33 C	−0.107	14 H	0.122	33 C	−0.274
15 O	−0.357	34 C	−0.249	15 O	−0.356	34 H	0.137
16 C	0.230	35 H	0.123	16 C	0.224	35 H	0.137
17 C	−0.099	36 H	0.131	17 C	−0.082	36 H	0.106
18 H	0.143	37 H	0.111	18 H	0.144	37 H	0.098
19 H	0.143	-	-	19 H	0.144	-	-


MBIF-1

MBIF-2

OIFB

NBIF

Figure 4. (Colour online) Mulliken atomic charge distribution.

slightly less absorption wavelength as compared to moderately attracting the cyano group.

Mulliken atomic charges for the molecules **MBIF-1** and **MBIF-2** are given in Table 10 and for the molecules **OIFB** and **NBIF** in Table 11. The Mulliken atomic charges of the title molecules are calculated by DFT/B3LYP method with a 6-311G (d,p) basis set in the gaseous phase. The pictorial representation of the Mulliken atomic charges given in Figure 4 uncovers that all hydrogen atoms have a net positive charge. The C16 (carbonyl carbon) and C6 carbon are highly electropositive. The H10 and H11 hydrogen atoms in all four molecules are highly electropositive in nature. The high electropositive character is a consequence of the hyperconjugation effect. In light of the vibrational frequencies, the different thermodynamic properties like total thermal energy (E_{total}), heat capacity at constant volume (Cv), total entropy (S), zero-point vibrational energy (Ev_0), rotational constants were computed. These are given in Table 12. It is evident from the data of E/B3LYP and E_{total} that the presence of electron releasing and electron attracting groups together augments the stability of the molecules. The **OBIF** molecule possesses highest stability. This is because of the presence of extended conjugation. The molecule **NBIF** has higher entropy amongst all the four molecules. This can be ascribed to the presence of more number of atoms in the molecule **NBIF**. The electron releasing groups (OR and

Table 11. Mulliken atomic charges of OIFB and NBIF molecules computed for B3LYP/6-311G (d,p) optimised geometries.

OIFB				NBIF			
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
1 C	−0.071	19 H	0.143	1 C	−0.063	19 H	0.147
2 C	−0.060	20 O	−0.322	2 C	−0.069	20 O	−0.314
3 C	−0.077	21 C	−0.148	3 C	−0.137	21 C	−0.216
4 C	−0.033	22 C	0.027	4 C	−0.028	22 C	0.025
5 C	−0.157	23 H	0.114	5 C	−0.148	23 H	0.108
6 C	0.250	24 C	−0.102	6 C	0.239	24 C	−0.094
7 H	0.115	25 C	−0.069	7 H	0.108	25 C	−0.026
8 H	0.094	26 C	−0.028	8 H	0.084	26 C	−0.100
9 C	−0.142	27 H	0.133	9 C	−0.166	27 H	0.112
10 H	0.140	28 H	0.110	10 H	0.143	28 H	0.108
11 H	0.136	29 C	−0.044	11 H	0.146	29 C	−0.018
12 C	−0.031	30 H	0.105	12 C	−0.013	30 C	0.117
13 H	0.122	31 C	−0.033	13 H	0.124	31 C	−0.034
14 H	0.115	32 H	0.117	14 H	0.124	32 H	0.138
15 O	−0.383	33 C	−0.059	15 O	−0.353	33 H	0.136
16 C	0.236	34 C	0.050	16 C	0.231	34 N	0.173
17 C	−0.099	35 N	−0.210	17 C	−0.101	35 O	−0.264
18 H	0.172	-	-	18 H	0.146	36 O	−0.265

Table 12. Thermodynamic properties.

Parameter	Value MBIF-1	 MBIF-2	 OIFB	 NBIF
E total (kcal mol^{-1})	197.278	198.009	179.906	182.734
Translational	0.889	0.889	0.889	0.889
Rotational	0.889	0.889	0.889	0.889
Vibrational	195.501	196.232	178.129	180.956
Heat Capacity at constant volume, Cv (cal mol^{-1}K^{-1})	65.851	67.675	67.775	70.415
Translational	2.981	2.981	2.981	2.981
Rotational	2.981	2.981	2.981	2.981
Vibrational	59.889	61.713	61.813	64.453
Total entropy S (cal mol^{-1}K^{-1})	132.255	136.519	136.881	142.423
Translational	42.746	42.953	42.862	43.062
Rotational	34.370	34.704	34.683	35.104
Vibrational	55.140	57.739	59.336	64.257
Zero point Vibrational Energy Ev$_0$ (kcal mol^{-1})	186.926	187.295	169.078	171.378
Rotational constants (GHZ)	1.097	0.910	1.079	0.879
	0.120	0.138	0.103	0.093
	0.109	0.120	0.094	0.084

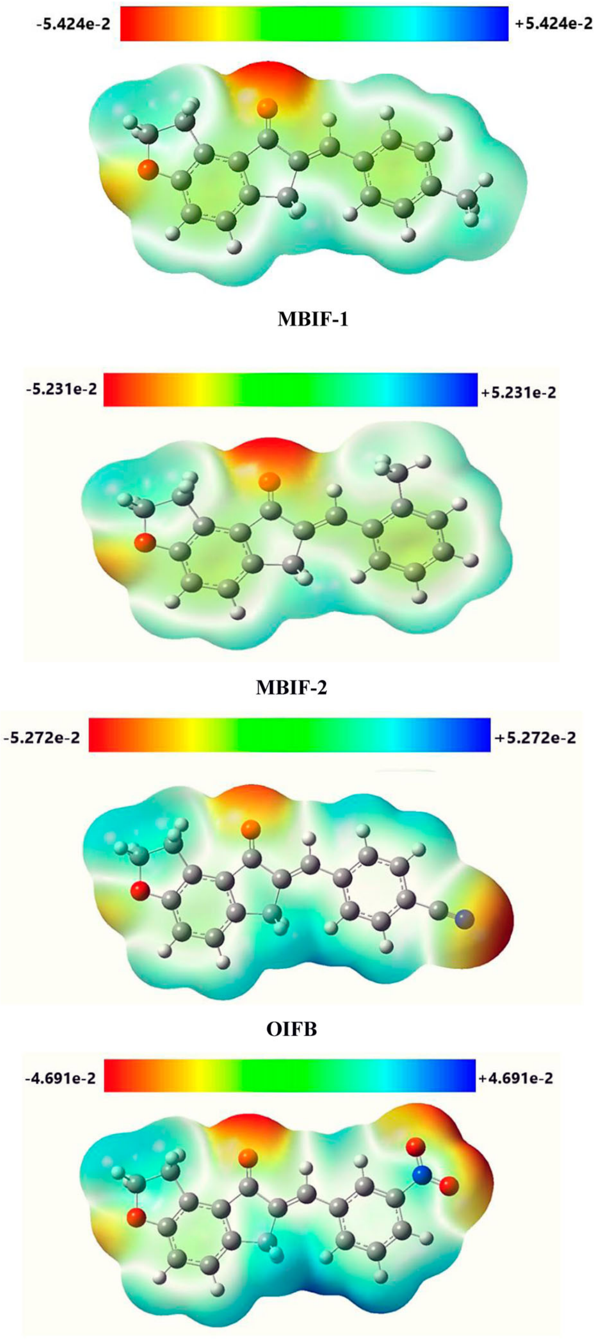


Figure 5. (Colour online) Molecular electrostatic potential surfaces.

Me) together results in the decrease in the stability of the molecules. The molecules **MBIF-1** and **MBIF-2** have nearly same more zero-point vibrational energy. All the thermodynamic data revealed is also valuable for additional assessment and can be utilised to figure the other thermodynamic energies.

The molecular electrostatic surface potential (MESP) plots are plotted by using a 6-311G (d,p) basis set and presented in Figure 5 MESP is the three-dimensional representation that indicates charge distributions in molecules. The properties like nucleophilic and electrophilic sites, solvent effects, hydrogen bonding interactions, etc. could be anticipated by understanding molecular electrostatic potential surfaces. The various estimations of the electrostatic potential at the surface of the molecule are represented by distinct colours. The red and yellow regions indicate the region of high electron density and are linked to electrophilic reactivity. On the other side, the blue parts represent low electron density and susceptible to nucleophilic reactivity and green colours represent regions of zero potential, respectively. The colour gradient ranges from most electronegative to the most electropositive are also displayed in the MESP plots. The surface around oxygen atoms is found to be the most electronegative red part. The most electronegative red part around oxygen atom is present in the **MBIF-1** molecule. The MBIF-1 molecule has colour gradient range from most electronegative to the most electropositive part as −0.05424 and +0.05424 respectively. This due to the presence of electron releasing methyl group in the **MBIF-1** molecule. The NBIF molecule has colour gradient range from −0.04691 to +0.04691. This is ascribed to the presence of powerful electron withdrawing group in the **NBIF** molecule. The electrophilic and nucleophilic sites give an idea regarding the area from where the compounds interact. The MESP suggests, in the title molecules, the aryl ring A connected to dihydrofuran ring is highly prone towards electrophilic attack. In the molecules **MIFB-1** and **MIFB-2**, ring A is more reactive towards electrophilic attack as compared to the ring A in molecules **OIFB** and **NBIF**. On the contrary, ring B in the molecules **OIFB** and **NBIF** are susceptible to the nucleophilic attack.

4. Conclusions

In conclusion, four new (*E*)-7-(arylidene)-1,2,6,7-tetrahydro-8*H*-indeno[5,4-*b*]furan-8-one derivatives are synthesised by the green method and studied from a structural examination perspective by using the DFT method with a basis set 6-311G (d,p). We have investigated the structural parameters along with global reactivity parameters for a better understanding of the stability and chemical behaviour of four important derivatives of the 7-arylidene indanone skeleton. Grindstone chemistry approach has been efficiently used for the synthesis of four new 7-arylidene indanones. The structures have been confirmed based on a ^{1}H NMR and ^{13}C NMR spectroscopic techniques. The geometry of the molecules was optimised by using a B3LYP/6-311G (d,p) basis set and the geometrical parameters like bond lengths and bond angles were computed at the same level of theory. The molecule NBIF has the highest polarity whereas the molecule MBIF-2 has the lowest polarity amongst all four molecules. The FMO study has been effectively presented to analyse the chemical reactivity of the molecules. The NBIF molecule has the lowest HOMO–LUMO energy gap amongst all molecules. By using HOMO–LUMO energies various electron and quantum chemical parameters have been established. The electron absorption energy information proposes that moving from electron releasing to electron attracting group on ring B brings about redshift. From the MESP analysis, it evident that in the molecules MIFB-1 and MIFB-2, ring A is more reactive towards electrophilic attack as compared to the ring A in molecules OIFB and NBIF. In contrast, ring B in the molecules OIFB and NBIF are susceptible to the nucleophilic attack. The OBIF molecule possesses higher stability while NBIF molecule has higher entropy.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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Collaboration/Linkage Certificate

TO WHOM IT MAY CONCERN

This is to certify that **Dr. Manohar Rajendra Patil** Department of Chemistry NTVS's G.T. Patil Arts, Commerce and Science College, Nandurbar-425412 has research collaboration (since 2017) with **Dr. Annapurna Jha, Head, Department of Chemistry, Jamshedpur Womens College, Jamshedpur, Jharkhand** for sharing the research ideas, exchange of reprints of our research papers and for the sample characterizations. We have jointly worked on research topics related to the application of nanoparticles and have published the research work in reputed international journals.

We have further extended this linkage with both the Chemistry departments to review the curriculum, teaching practices and discuss ways in which courses could be revised to promote scientific knowledge among the students.

Date: 01/09/2017

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Enhance catalytic performance of lipase immobilized on Polyaniline (PANI)–Fe3O4 magnetic nanocomposite and its application in biodiesel synthesis from waste cooking oil

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Abstract:	Biodiesel is recently used as a substitute for petroleum based diesel due to environmental considerations and depletion of vital resources like petroleum and coal. In the present work biodiesel was synthesized by immobilized lipase to make the process cost effective. Lipase was immobilized on magnetic nanocomposite which can be easily separated from the reaction medium by magnetic separation. In the present investigation lipase was immobilized on modified polyaniline (PANI)–Fe3O4 magnetic nanocomposite. SEM images demonstrate the morphology of modified nanocomposite with and without immobilized lipase. The modified nanocomposites with and without immobilized lipase were further characterized with Thermogravimetric analysis (TGA) and Fourier Transform Infrared (FTIR) Spectroscopy. At higher temperature the immobilized lipase was more stable in comparison to its free form. Immobilized lipase retained 84% of its initial activity on incubation at 90 0C whereas free form became inactive at this temperature. The optimum pH shifted from 7 for free lipase to 8 for the immobilized lipase. The conversion yield of biodiesel was found to be 80% with the immobilized lipase while it was only 28% with free lipase. Immobilized lipase can be reused for 5 cycles with 90% retained activity for biodiesel synthesis. Immobilization of lipase on polyaniline (PANI)–Fe3O4 magnetic nanocomposite improved its stability towards denaturation by heat and pH. Moreover it has quite efficiently catalyses the biodiesel synthesis with good operational stability.
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Journal of the Indian chemical Society

Subject: - Submission of an original research article

Dear editor,

I would like to submit the manuscript entitled “Enhance catalytic performance of lipase immobilized on Polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite and its application in biodiesel synthesis from waste cooking oil” to be considered for publication as original article in your esteemed journal the “Journal of the Indian chemical Society”.

We declare this submission has not been previously published in English or in other language.

We declare that this manuscript is original and is not currently being considered for publication elsewhere.

The authors do not have any conflict of interests to declare.

This article is not based on a conference paper.

As corresponding author I confirm that manuscript has been read and approved for submission by all the authors.

Please address all correspondence concerning this manuscript to me at annujha05@gmail.com.

Thank you for your consideration of this manuscript.

Sincerely,

Dr. Annapurna Jha

Enhance catalytic performance of lipase immobilized on Polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite and its application in biodiesel synthesis from waste cooking oil

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Abstract

Biodiesel is recently used as a substitute for petroleum based diesel due to environmental considerations and depletion of vital resources like petroleum and coal. In the present work biodiesel was synthesized by immobilized lipase to make the process cost effective. Lipase was immobilized on magnetic nanocomposite which can be easily separated from the reaction medium by magnetic separation. In the present investigation lipase was immobilized on modified polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite. SEM images demonstrate the morphology of modified nanocomposite with and without immobilized lipase. The modified nanocomposites with and without immobilized lipase were further characterized with Thermogravimetric analysis (TGA) and Fourier Transform Infrared (FTIR) Spectroscopy. At higher temperature the immobilized lipase was more stable in comparison to its free form. Immobilized lipase retained 84% of its initial activity on incubation at 90 ^{0}C whereas free form became inactive at this temperature. The optimum pH shifted from 7 for free lipase to 8 for the immobilized lipase. The conversion yield of biodiesel was found to be 80% with the immobilized lipase while it was only 28% with free lipase. Immobilized lipase can be reused for 5 cycles with 90% retained activity for biodiesel synthesis. Immobilization of lipase on polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite improved its stability towards denaturation by heat and pH. Moreover it has quite efficiently catalyses the biodiesel synthesis with good operational stability.

Keywords: PANI–Fe3O4 magnetic nanocomposites, Lipase, Immobilization, Thermostability, Biodiesel

1.Introduction:

Biodiesel syntheses from vegetable oils have immense potential as a renewable source of energy. A number of processes have been developed for biodiesel production involving chemical or enzyme catalysis or supercritical CO_2 medium [1][2][3]. Enzymatic transesterification of triglycerides is a good alternative to chemical process as it is a green approach of producing renewable fuel. Enzyme catalysis has shown high purity of products due to its ecofrienldly, selective nature and low temperature requirement [2].

In many countries biodiesel synthesized using edible and non-edible oil; however because of the high cost of the vegetable oils biodiesel cost 1.5 times higher than fossil diesel and it limited its wide application[3]. Therefore in the present study, waste oils chosen as the raw materials for biodiesel synthesis.

There are many reports on biodiesel production using enzyme catalysis by free or immobilized lipase. Immobilized lipase in particular is suitable for continuous biodiesel production because of its ease of recovery from the reaction mixture. A great variety of lipase immobilisation methods such as adsorption, covalent immobilization, entrapment and whole-cell biocatalyst have been reported [4][5]. Among the various immobilization methods adsorption and covalent immobilization methods are the most cost effective and efficient means of immobilization. Adsorption is one of the easiest methods but the bonding of the enzyme to the matrix is often weak and such biocatalysts generally lack the degree of stabilization achieved by covalent attachment. Covalent immobilization methods have the strongest enzyme-support bonding compared with other methods. The lipase needs both firmness and flexibility, as the flexible active center enhances its endurance towards distortions without losing activity. But strong multipoint covalent bonding will lead to the irreversible distortion of active center and the risk of losing function. So in the present investigation an intermediate process between adsorption and covalent attachment has been utilized for immobilization of *Aspergillus niger* (RM1265) lipase to enhance the immobilization efficiency and stability of enzyme.

Lipases immobilized on nanoparticles are an excellent catalyst for biodiesel synthesis [6]. The magnetic nanocomposite has been utilized for immobilization as the smaller size particles will increase the total acting surface of reacting particles in reaction mixture, moreover magnetic isolation of lipase make the processes is advantageous from an economic point of view. In the present investigation, *Aspergillus niger* (RM1265) lipase was first immobilized on activated nanocomposite then it was utilized for methanolysis of waste oil.

2. Experimental:

2.1. Chemicals

Lipase from *Aspergillus niger* (RM1265) was purchased from HiMedia and *p*-nitrophenol palmitate was purchased from Sigma aldrich. Waste cooking oil was collected from local restaurants. All other solvents and reagents were AR grade.

2.2. Modification of nanocomposite

Polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite has been utilized for immobilization of lipase which was synthesized in situ through self-polymerization of monomer aniline [7]. 5g magnetic nanocomposites were modified by refluxing it in 25 ml ethanolamine. After 3 h of reflux nanocomposite were washed thrice with 60 ml acetone and air dried. Magnetic nanocomposites were then activated using 25 ml 4% (w/v) glutaraldehyde in 50 mM phosphate buffer (pH 8.0) with gentle agitation at 4 ^{0}C for 2 h. The activated magnetic nanocomposites were washed with phosphate buffer to make it glutaraldehyde free.

2.3. Immobilization of lipase

About 25 ml lipases in 50 mM phosphate buffer (pH 8.0) was mixed with 0.1 ml of Tween 80 and stirred for 5 min followed by the addition of 5 g of magnetic nanocomposite. Hundred milliliter of chilled acetone was added and the mixture was stirred for 30 min at 4 ^{0}C. Magnetic nanocomposite immobilized lipase was filtered, washed with 25 ml of chilled acetone and lyophilized.

2.4. Lipase assay

Lipase assay was done spectrophotometrically using *p*-nitro phenyl palmitate as the substrate[8]. One unit (U) of lipase was defined as the amount of enzyme that liberates 1 µmol of p-nitro phenol per min under the assay conditions.

2.5. *Characterizations of immobilized lipase*

2.5.1. *SEM analysis*

SEM analysis of modified nanocomposite and lipase immobilized modified nanocomposite were carried out on using HITACHI-S- 4800(type II) instrument, Japan.

2.5.2. ***Thermo Gravimetric Analysis:*** TGA of modified nanocomposite and lipase immobilized modified nanocomposite were carried out using Thermal analyser -Perkin Elmer Pyris -1 TGA.

2.5.3. ***FTIR Analysis:*** FTIR analysis of modified nanocomposite and lipase immobilized modified nanocomposite were carried out on FT-IR Spectrometer Perkin Elmer Spectrum GX 10,000 cm^{-1} to 370 cm^{-1}.

2.5.4. *Effect of temperature and Thermostability*

The effect of temperature on the free and immobilized lipase activity was determined for *p*-NPP hydrolysis. The hydrolysis of *p*-NPP was observed at various temperatures (20–70^{0}C), where the *p*-NPP solution was preincubated to reach the desired temperature before the addition of lipase.

2.5.5. *pH stability and Thermostability*

The effect of pH on the free or immobilized enzymes was examined after pre-incubating the enzyme samples at 30^{0}C for 60 min at pH 4–11 [50 mM sodium acetate buffer (pH 4, 5), 50 mM potassium phosphate buffer (pH 6,7), 50 mM Tris–HCl buffer (pH 8, 9), and 50 mM glycine–NaOH buffer (pH 10, 11)]. Then the residual activity was assayed under the standard conditions. Thermostsbility of the free and immobilized lipase activity was observed by incubating in phosphate buffer (50 mM, pH 7.0) at temperatures ranging from 30°C to 90°C for 60 min, followed by measurement of the residual enzyme activity at 37°C. The enzyme activity of the not incubated lipase was taken as 100%.

2.6. Biodiesel synthesis

2.6.1. Reaction setup for transesterification reaction

Transesterification reaction for biodiesel synthesis was carried out at 30°C in screw-capped vials placed inside a reciprocal shaker. The initial reaction mixture consisted of oil: methanol molar ratio of 1:2, *t*- butanol:oil volume ratio of 0.2, immobilized lipase 50 U and 200 rpm along with the respective controls (samples without enzyme).

2.6.2. Sampling and Analysis

Synthesis of fatty acid methyl ester was analyzed by method was modified based on hydroxamic acid test [9].

2.7. *Operational stability of nanocomposite bound lipase*

Operational stability of immobilized lipases was also observed for biodiesel synthesis. After the completion of reaction, the immobilized lipases were collected by centrifugation at 5,000 rpm for 10 min and washed with hexane in order to remove the reactants adsorbed on matrix. Then the immobilized lipases were resuspended in the same composition of freshly prepared reaction mixture to start a new run and the supernatant was assayed for biodiesel synthesis.

3. Result and discussion:

3.1. Immobilization of enzyme

Immobilization of lipase was carried out on modified crosslinked nanocomposite, where the immobilization yield of lipase on was estimated by calculating the specific activity of respective lipases before and after binding to nanocomposite. Lipase showed 85% immobilization on modified cross linked aminated nanocomposite. The present result of immobilization yield is higher than those earlier reports [10][11]. Covalent attachment is the most efficient method of enzyme immobilization, but because of strong multi-interactions between the enzyme and support, sometimes distortions of enzymes occur that lead to denaturation and loss of enzyme activity. In the present immobilization process first ethanolamine was adsorbed on nanocomposite and then it was treated with glutaraldehyde followed by enzyme immobilization. So this process is not completely covalent attachment therefore lipase is efficiently immobilized on activated nanocomposite without losing its enzyme activity. It was observed that the activated nanocomposite enhances the immobilization yield and thermostability of lipase.

3.2. SEM analysis of modified nanocomposite and lipase immobilized on modified nanocomposite

Scanning electron microscopy is widely used to study the morphological features and surface characteristics of catalyst surface. The magnetic nanocomposite of Polyaniline/Fe_3O_4 are analyzed by SEM after activation with ethanolamine and glutaraldehyde as shown in Figure(1a**)**. In Figure(1a**)** polyaniline–Fe_3O_4 has heterogeneous surface, there is whitish cluster of Fe_3O_4 nanoparticles on the dark greyish surface of polyaniline that we have used earlier for degradation of dyes[7]. The SEM micrographs of magnetic nanocomposite of polyaniline/Fe_3O_4 also showed surface texture and porosity in figure 1(a).The magnetic nanocomposite of polyaniline/Fe_3O_4 are analyzed by SEM after the enzyme immoblisation as shown in Figure 1b. The figure 1(b) shows increased in surface texture and porosity, that's mainly due to successfully binding of the enzyme substrate with the surface. So, we easily distinguished figure 1(a) and 1(b) from their porosity and concluded successful enzyme immobilisation on modified polyaniline/ Fe_3O_4 catalyst nanocomposite.

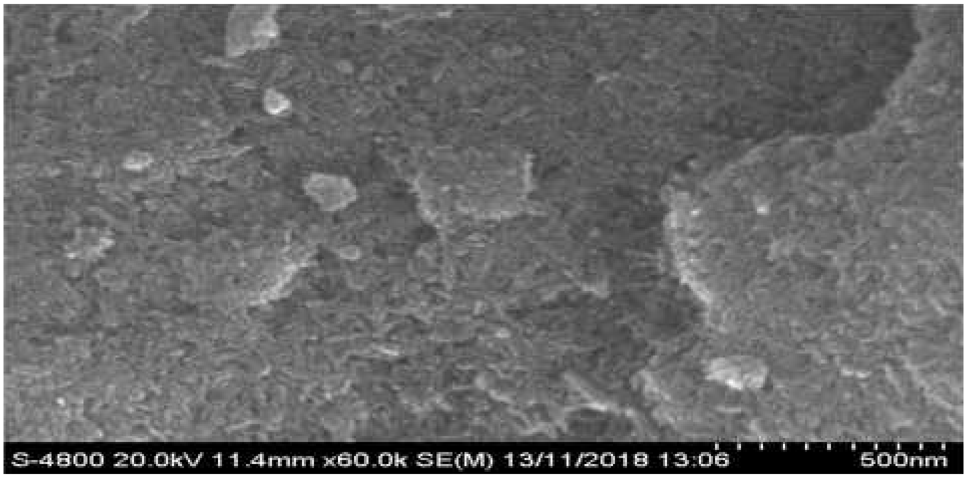

Figure 1a: SEM of magnetic nanocomposite of polyaniline/Fe_3O_4 modified after treatment with ethanolamine and glutaraldehyde

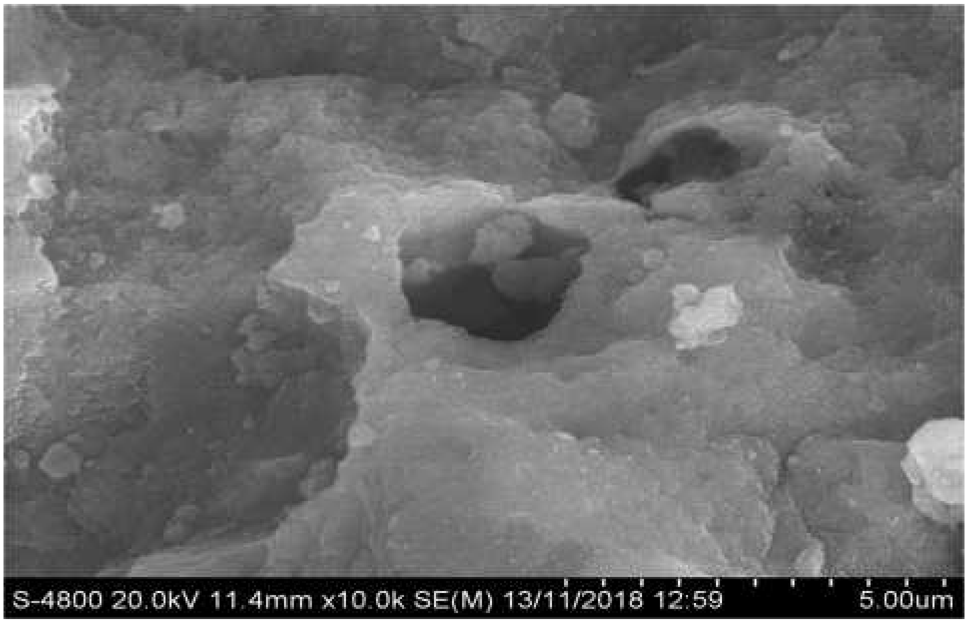

Figure 1b: SEM of lipase immobilized modified magnetic nanocomposite of polyaniline/Fe_3O_4.

3.3. TGA of activated nanocomposite and lipase immobilized on activated nanocomposite

Thermogravimetric analysis (TGA) is very practical tool to extract structure-related information of the materials. In present investigation thermal analyses reveal that the modified polyaniline and enzyme immobilized polyaniline are thermally labile materials, as shown in figure 2a and 2b. The initial weight loss around 200 ^{0}C was mainly due to evaporation of water and low molecular weight species. The second weight loss 220 to 300 ^{0}C was associated with the doping agent degradation. The weight loss around 400 to 500 ^{0}C was associated with degradation of polyaniline. Beyond 500 ^{0}C Fe_3O_4 was decomposed from covalently bonded Polyaniline. This trend was observed in both the Figure 2a (Polyaniline- Fe_3O_4) and Figure 2b (Polyaniline- Fe_3O_4 enzyme nanocomposite). But weight loss is slightly more in Figure 2b that is due to use of enzyme in a reaction.

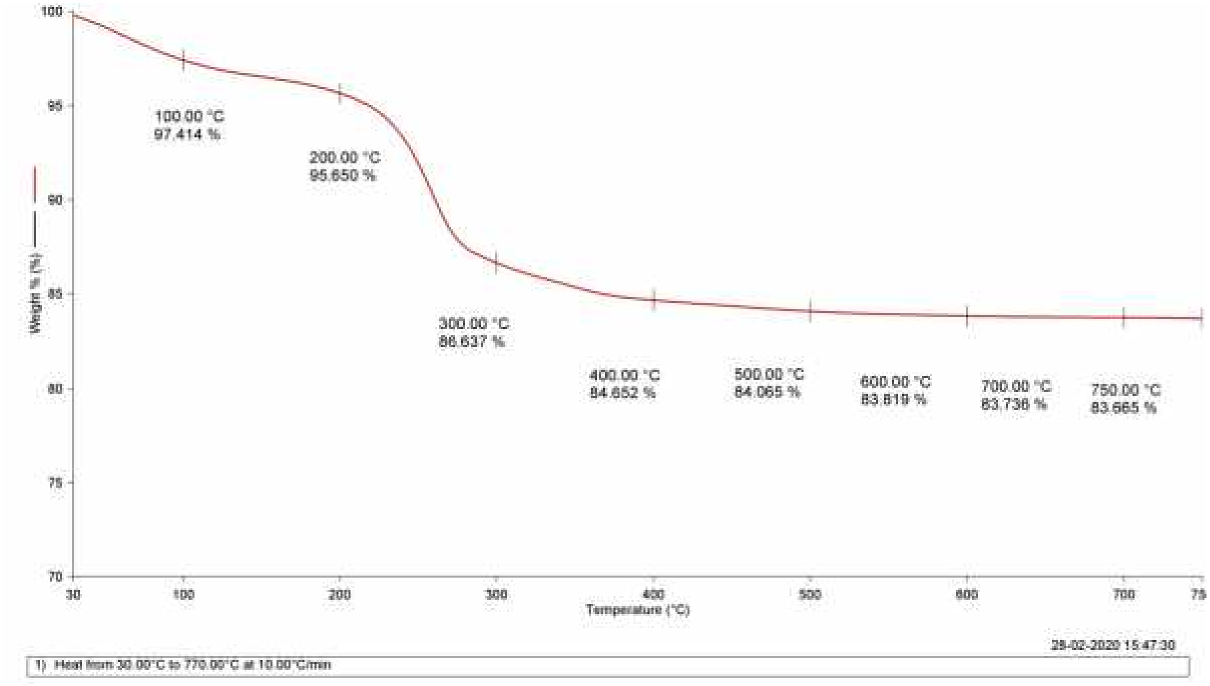

Figure 2a: TGA curve of magnetic nanocomposite of polyaniline/Fe_3O_4 modified after treatment with ethanolamine and glutaraldehyde

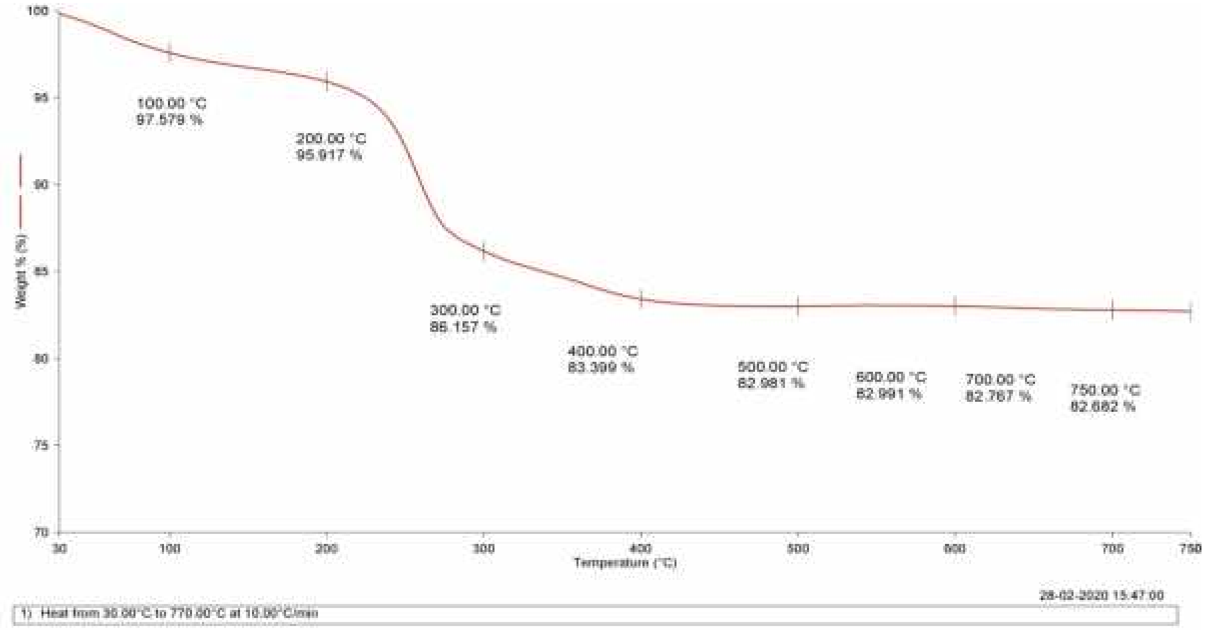

Figure 2b: TGA curve of lipase immobilized modified magnetic nanocomposite of polyaniline/Fe_3O_4.

3.4. FT-IR analysis of activated nanocomposite and lipase immobilized on activated nanocomposite

The FT-IR spectra of activated PANI–Fe_3O_4 nanocomposite and enzyme immobilized PANI–Fe_3O_4 nanocomposite are shown in figure 3a and 3b respectively. It shows absorption band at 468 cm^{-1}, due to Fe–O stretching vibration. The peaks found at 3408, 1112 and 1070 may be assigned to N–H stretching and C–N stretching vibration respectively. The peak appeared at 1633 and 1620 cm^{-1} are due to C=C stretching vibration in aromatic ring of aniline. Almost all the peaks are common in both the Figure 3a and Figure 3b except for peak at 2854 cm^{-1} which may assigned to C-H stretching vibration of aldehyde group. This is because activated PANI–Fe_3O_4 nanocomposite has free aldehyde group which is utilized for lipase immobilization in enzyme immobilized PANI–Fe_3O_4 nanocomposite. So FTIR analysis showed the efficient enzyme immobilization on PANI–Fe_3O_4 nanocomposite.

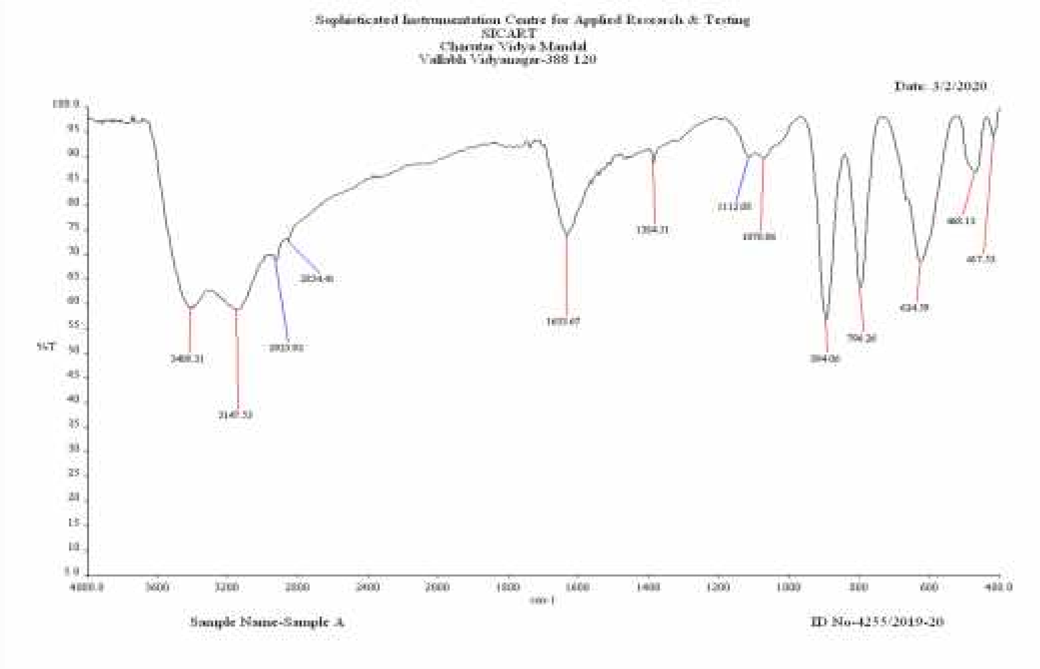

Figure 3a: FTIR spectrum of magnetic nanocomposite of polyaniline/Fe_3O_4 modified after treatment with ethanolamine and glutaraldehyde.

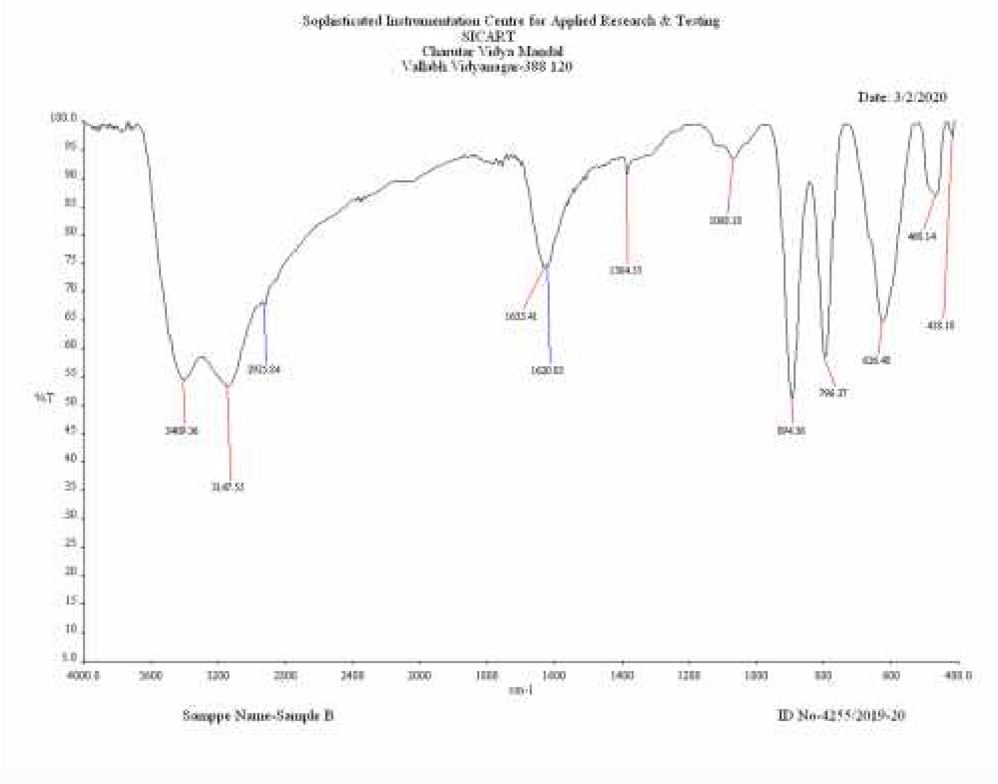

Figure 3b: FTIR spectrum of lipase immobilized modified magnetic nanocomposite of polyaniline/Fe_3O_4.

3.5. Effect of temperature on lipase activity

Application of lipases in chemical synthesis, especially biodiesel production, often leads to thermal inactivation due to denaturation of the protein. Figure 4 illustrates the effect of temperatures on free as well as immobilized enzyme. It has been observed that the free and immobilized lipases had almost same activity up to 40 ^{0}C while at higher temperature the immobilized lipases were more stable and showed a slight increase in activity. This may be because immobilization of enzymes by multiple point binding resulted in an increase of enzyme rigidity, which is commonly reflected by increase in stability towards thermal denaturation. This result is in consistent with earlier reports [11].

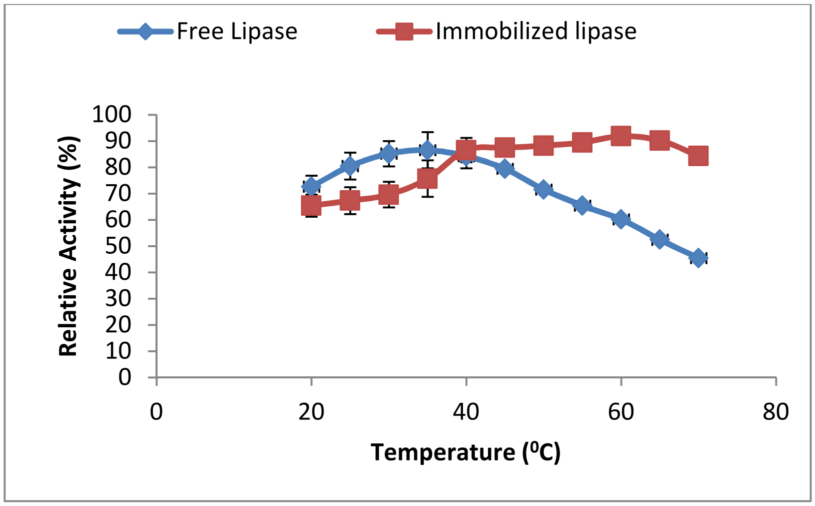

Figure 4: Effect of temperature on free and immobilized lipase. Data are represented as the mean ± standard deviation of three replications.

3.6. Thermostability of free and immobilized lipases

Thermal stability of an enzyme has immense importance for its potential industrial applications. The thermal stability of immobilized enzymes used to increase on attachment to a rigid support. In the present study thermal stability of the soluble and immobilized lipase was studied at various temperatures from 30^{0}C to 90^{0}C (Figure 5). It was observed that free lipase activity decreased after 40^{0}C and became inactive beyond 60^{0}C while the immobilized lipase was completely retained its activity. It has been observed that even at 90^{0}C, after one hour of incubation, the immobilized lipase retained 84% of its initial activity, whereas the free lipase became inactive far before this temperature. Although there are several previous reports where immobilized lipase was stable in comparison to its free form but the thermal stability observed in the present study was found to be very much improved than the earlier reports [12] [13].

Thermal stability depends on the strength of bonds formed between the enzyme and the support which prevent its unfolding at higher temperature. The thermal stability of immobilized enzymes might be drastically increased due to its strong attachment to activated magnetic nanocomposite.

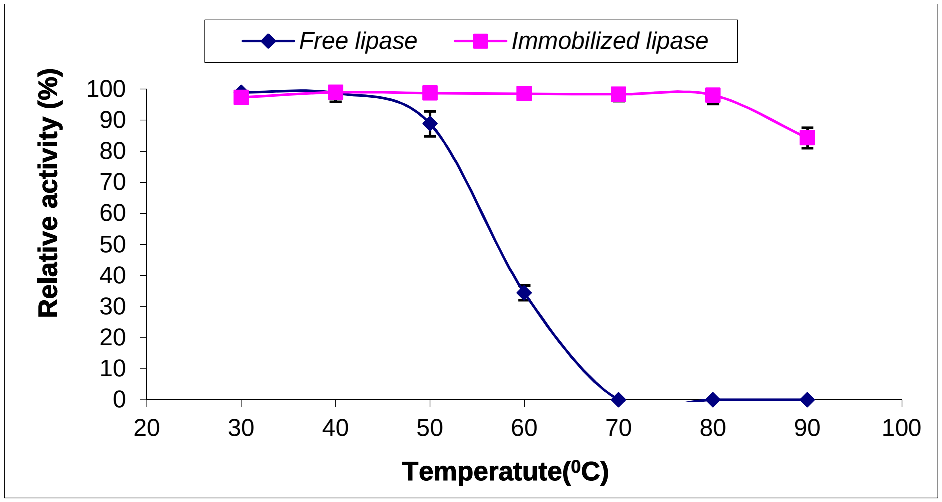

Figure 5: Thermostability of free and immobilized lipase. Data are represented as the mean ± standard deviation of three replications.

3.7. Effect of pH on lipase activity

Immobilization of enzyme may attribute to the conformational changes of enzyme resulting in a variation of optimum pH. According to the present observation free as well as immobilized lipases remained stable in the pH range from 4 to 7. pH 8 onwards immobilized lipase retained activity, while free lipase started deactivating (Figure 6). This higher stability of immobilized lipase may be due to the bonding between enzyme and activated magnetic nanocomposite, which prevent the denaturation of enzyme at basic pH [14].

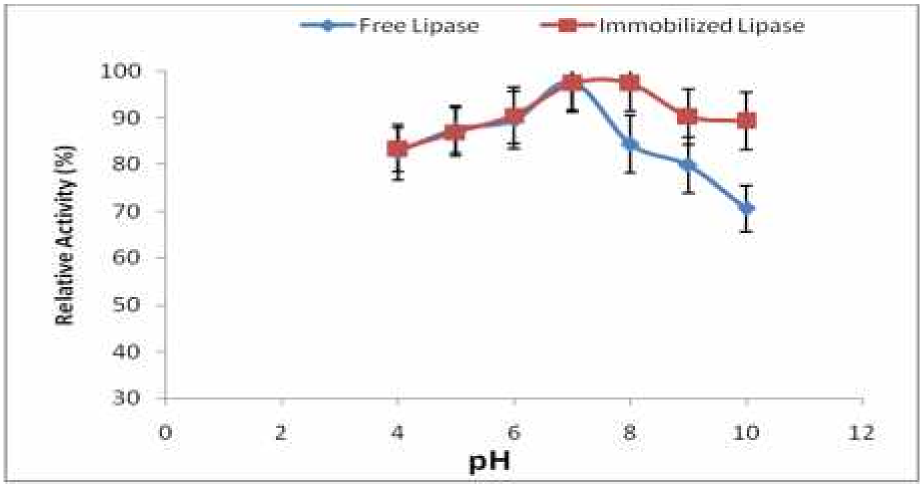

Figure 6: Effect of pH on free and immobilized lipase. Data are represented as the mean ± standard deviation of three replications.

3.8. Kinetic parameters of free and immobilized lipases

The kinetic constants Vmax and Km were calculated from the double reciprocal plots shown in Figure 7. Free lipase showed Km values of 0.4mM and Vmax 1.5 U/mg, while immobilized lipase had Km value of 0.27 mM and Vmax 1.4 U/mg. The decrease in km value showed that immobilization had increased the affinity of enzyme for the substrate, which was in agreement with those obtained previously [15][16]. In general, Vmax values of enzymes exhibit a decrease on immobilization; which is in accordance with the other similar results [15].

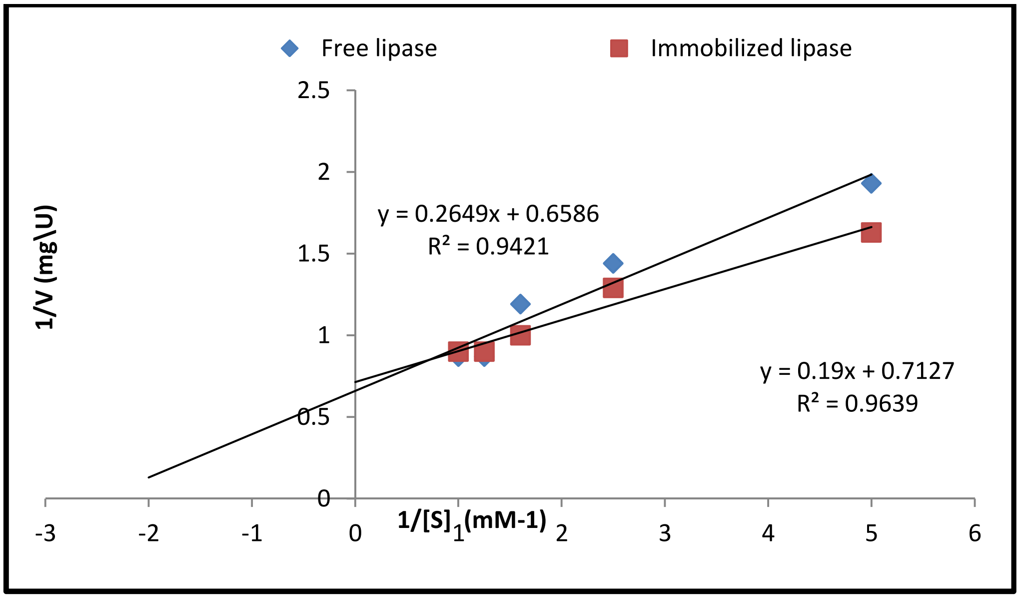

Figure 7: Lineweaver–Burk plots for free and immobilized lipase

3.9. Synthesis of biodiesel by free and immobilized lipases

The capacity of the immobilized and the free lipases to catalyze biodiesel synthesis in solvent free system was investigated (Figure 8). The results showed that a higher percentage conversion of 80% was obtained with the immobilized lipase; however, the conversion percentage does not exceed 28% using the free lipase after 30h of reaction time. This result was found to be improved than those earlier reported ones [17]. The enhanced efficiency of immobilized lipase for biodiesel synthesis may result from multipoint attachment between lipase and the activated nanocomposite, which prevents distortions of enzymes in reaction mixture.

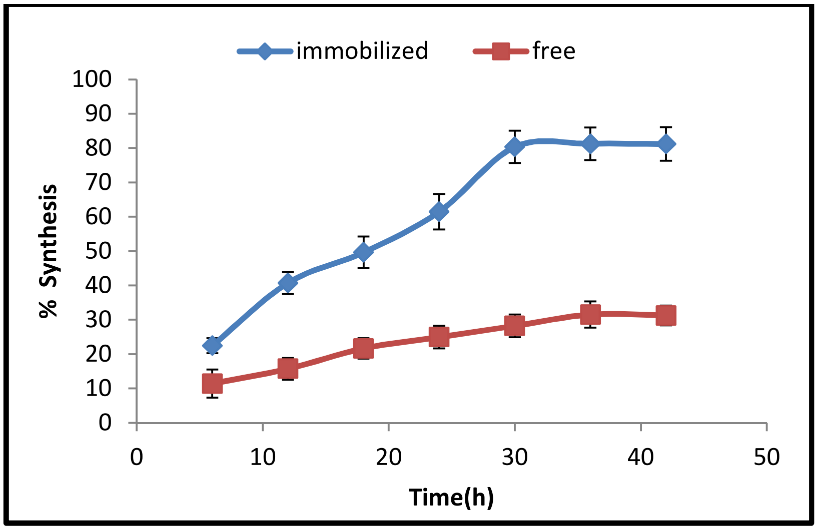

Figure 8: Biodiesel synthesis with free and immobilized lipase. Data are represented as the mean ± standard deviation of three replications.

3.10. Operational stability of immobilized lipases

As a potential industrial enzyme, operational stability of the immobilized lipase is very important parameter for the economy of the process. Immobilized lipase could be reused up to five cycles, with almost 90% retention of its original activity (Figure 9), which is found to be improved when compared with the other reports[18][19][20]. The good operational stability may be due to the strong interaction between enzyme and the matrix. The strong interaction can be further attributed to the formation of Schiff’s base between free aldehyde groups of glutaraldehyde treated nanocomposite and the side-chain amino groups of the enzyme. Significant stability of lipase immobilized on nanocomposite in organic solvent ensured good reuse capacity for biodiesel synthesis.

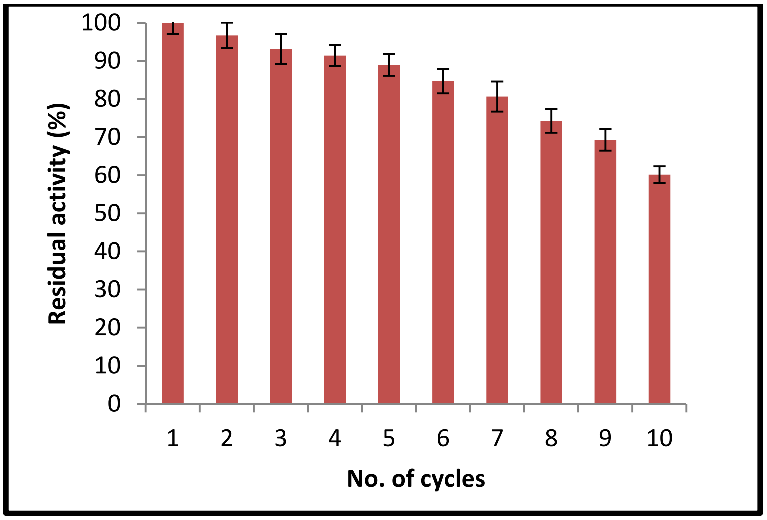

Figure 9: Operational stability of immobilized lipases for biodiesel synthesis. Data are represented as the mean ± standard deviation of three replications.

Conclusion:

Immobilization of lipase has been attempted successfully on polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite activated with ethanolamine followed by cross linking with glutaraldehyde. Immobilization has been carried out using adsorption technique that causes less damage to the catalytic activity of the enzyme. In the present investigation it has been seen that the immobilized lipases exhibited quite improved tolerance against thermal denaturation than free forms. The use of thermostable enzymes in chemical reactions to be performed at higher temperature leads to completion of reaction in shorter times. The immobilized lipases also showed enhanced activities for biodiesel synthesis than free forms, which undoubtedly explain the rationale for using immobilized lipase in organic synthesis. Furthermore, the immobilized lipase also exhibited quite well operational stability for biodiesel synthesis. Altogether, these results confirmed that the polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite is a potential support in the enzyme immobilization technology especially for catalyzing reactions in organic media.

Consent for publication

Not applicable.

Funding

None.

Conflict of interest

The author declares that there is no conflict of interest, financial or otherwise.

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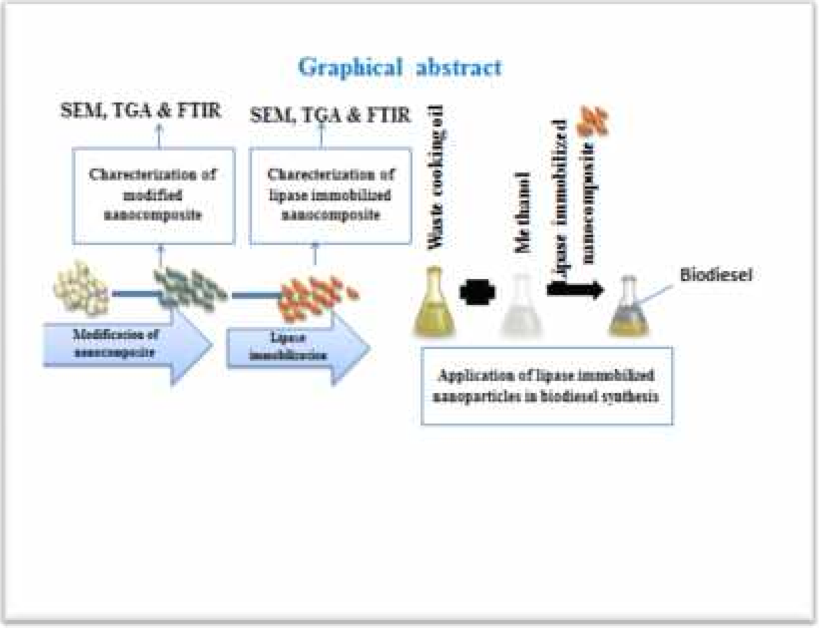
Graphical abstract
SEM, TGA & FTIR
SEM, TGA & FTIR
Charecterization of modified nanocomposite
Charecterization of lipase immobilized nanocomposite
Modification of nanocomposite
Lipase immobilization
Waste cooking oil
Methanol
Lipase immobilized nanocomposite
Biodiesel
Application of lipase immobilized nanoparticles in biodiesel synthesis

Declaration of Interest

Research Highlights

- Lipase has been immobilized on magnetic nanocomposite (modified polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite) which can be easily separated from the reaction medium by magnetic separation.
- SEM was carried out to study the morphology of modified nanocomposite with and without immobilized lipase.
- Modified nanocomposites with and without immobilized lipase were also characterized with Thermogravimetric analysis (TGA) and Fourier Transform Infrared (FTIR) Spectroscopy.
- Immobilized lipase was found to be more thermostable than its free form.
- The optimum pH and temperature for the immobilized lipase on modified polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite were also studied.
- The conversion yield of biodiesel was found to be 80% with the lipase immobilized on modified polyaniline (PANI)–Fe_3O_4 magnetic nanocomposite while it was only 28% with free lipase.

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Synthesis of Magnetic Nano Sized Cobalt Ferrite Thin Film by Chemical Bath Deposition Method and their Photocatalytic Application for Removal of Congo red Dye

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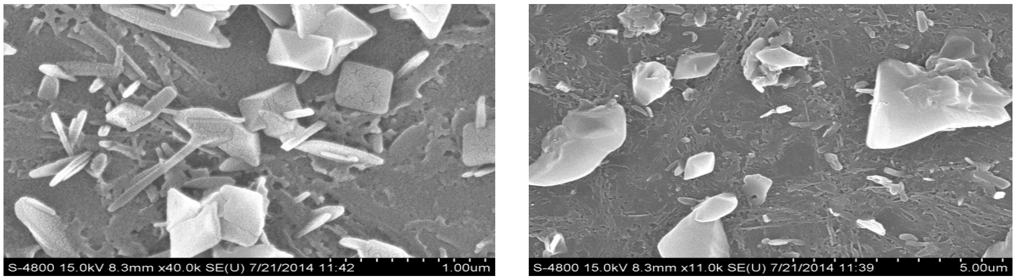
ABSTRACT

The present investigation report is a novel method for the removal of Congo red (CR) dye from an aqueous solution. In present investigation cobalt ferrite ($CoFe_2O_4$) thin film was deposited on glass substrate by using chemical bath deposition method. It was successfully prepared while nanostructure of thin film was confirmed by SEM and XRD characterization method. The magnetic property of the film was confirmed by VSM (Vibrating sample magnetometer). The average crystal size calculated by Scherrer formula from XRD analysis is 28 nm. Prepared thin film was then applied for photocatalytic degradation of Congo red dye by dipping it in aqueous solution. Different parameters like contact time, different initial conc. and pH have been studied to optimize reaction condition. The optimum conditions for the removal of the dye are initial concentration 30 mg L^{-1}, contact time 120 min and pH 7.

Graphical Abstract



SEM micrograph of prepared $CoFe_2O_4$ thin film

Keywords: Congo red dye, cobalt ferrite, SEM and XRD, VSM.

INTRODUCTION

Azo dyes are synthetic dyes, having an azo group (-N=N-) in the structure. Azo dyes are commonly utilized for dyeing textiles and leather. Some azo dyes may engender carcinogenic aromatic amines under certain conditions [1]. Most of those colored dyes are synthetic in nature and are conventionally composed of aromatic rings in their molecular structure, which makes them carcinogenic, mutagenic, inert, and non-biodegradable when discharged into aqueous streams without felicitous treatment. Therefore, the abstraction of such colored agents from the polluted aqueous stream is very exigent predicated on the point of human health and environmental resource auspice [2, 3].

Chemical bath deposition (CBD) is a very simple method has been used for preparation of Nano thin films. In this method only important thing is to maintain proper condition for the preparation of thin films. Several researchers have been using this method for the preparation of Nano thin films [4-10].

Photocatalytic degradation of organic pollutants especially dyes are carried out using catalyst in powder form. But during the recovery of this catalyst after experiment loss takes place. To overcome this shortcoming best alternative is use of thin film for the degradation of dyes. By using thin films several researchers have carried photocatalytic removal of pollutants [11-16].But in this report we have used magnetic nano thin film which is very different from other researcher work.

MATERIALS AND METHODS

All chemicals used were analytical grade. The stock solution 1000 mgL^{-1} of dye was prepared in distilled water. 100 mL of dye solution of the desired concentration was prepared from stock solution. In 100 mL of Congo red dye solution of a different concentration prepared thin film is dipped. Then dipped thin film, dye solution was irradiated with mercury lamp to provide energy to excite $CoFe_2O_4$ thin film molecule in the reactor. At specific time intervals suitable aliquot of the sample is withdrawn and analyzed after centrifugation. The changes of dye concentration are determined by UV-Visible double beam spectrophotometer (Systronics model-2203) at λ max 510 nm in our laboratory.

Synthesis: Alkaline bath for cobalt ferrite thin films was prepared by A.R. grade chemicals using double distilled water. Bath consist of 0.1 M solution of $CoCl_2$ $6H_2O$ and 0.2 M solution of $FeCl_3$ $6H_2O$. These salts were used as source of Co^{+2} and Fe^{+3}ions by adding NH_4OH solution made the bath alkaline up to pH-11. The deposition of film was carried out on glass substrate. The glass substrate etched with 2 % dilutes HCl for approximately 20 Sec and ultrasonically cleaned with double distilled water. Finally substrate was dried in air.

The washed and dried glass substrate was immersed in combined alkaline cobalt (II) chloride and iron (III) chloride solution bath. When bath attains the temp of 70°C the precipitate of mixed solution was settled. During the precipitation heterogeneous reaction occurred on the substrate and deposition of cobalt ferrite takes place on the substrate. The film formation started after about 10 min and completed in 120 min at 70°C. Cobalt and iron hydroxides adsorbed onto the substrate during the process.

$$CoCl_2 + 2FeCl_3 + 8\ NH_4OH \rightarrow CoFe_2O_4 + 8\ NH_4Cl + 4H_2O$$

Then this film is dried in hot air and annealed at 500° C for 4 h to form pure cobalt ferrite with cubic Spinel phase, removing any hydroxide content and complete crystallization of the film takes place.

RESULTS AND DISCUSSION

X-ray Diffractometry (XRD): The XRD diagram of $CoFe_2O_4$ is as shown in fig-1.It shows main peak at 35.58^0 and subsidiary peak at 43.73^0, 64.45^0. It shows match scan with **JCPDS card NO-221086** at radiation of 1.54 A^0.The intensity of peaks indicates the crystallinity of $CoFe_2O_4$.The average particle size of $CoFe_2O_4$ is estimated by Scherer formula is 28 nm.

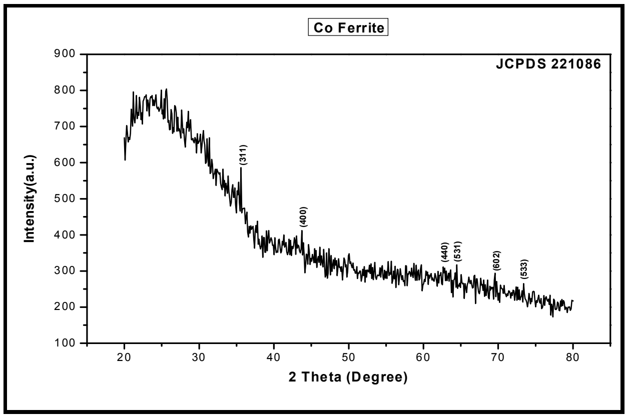


Figure 1. XRD analysis of prepared $CoFe_2O_4$ thin film.

Scanning electron microscopy (SEM): The $CoFe_2O_4$ Nano thin film is analyzed by SEM before fig 2(a) and after photocatalytic degradation of CR dye is shown in the fig 2(b). It shows SEM micrographs of $CoFe_2O_4$. Fig-2(a) shows surface texture and whitish cluster on $CoFe_2O_4$ thin film. It has homogeneous surfaced, some microspores as seen from its surface micrographs. It is black-whitish in color, Fig-2 (b) shows after photo degradation of CR on $CoFe_2O_4$ surface. The thin film surface is similar to before photocatalytic degradation.

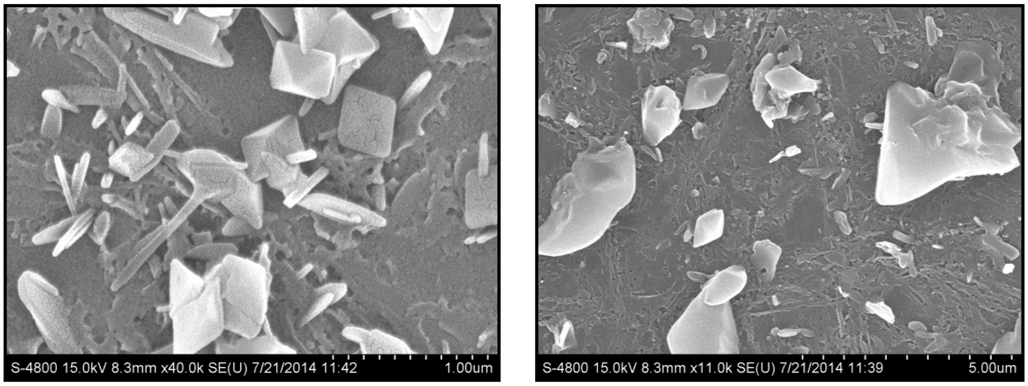


Figure 2. (a) and (b) SEM micrograph of prepared $CoFe_2O_4$ thin film

Vibrating sample magnetometer (VSM) Analysis: The magnetic property of $CoFe_2O_4$ Nano thin film was analyzed at R.T by VSM (Vibrating sample magnetometer) at an applied field of 10,000 Gauss. The value of saturation magnetization is 36.5 emu g^{-1}. It is shown in the curve of the fig 3. So this magnetization curve of the sample shows a ferromagnetic behavior, with hysteresis. The magnetic property of nanocomposite is dependent on the sample shape, crystallinity; therefore it can be adjusted to obtain optimum property.

Parametric Studies: The photocatalytic degradation of Congo red dye was studied at λ max 510 nm. The utmost condition for removal of dyes is 30 mg L^{-1}, pH 7 and prepared $CoFe_2O_4$ thin film. The results obtained during this study are represented in (Fig 4-6).

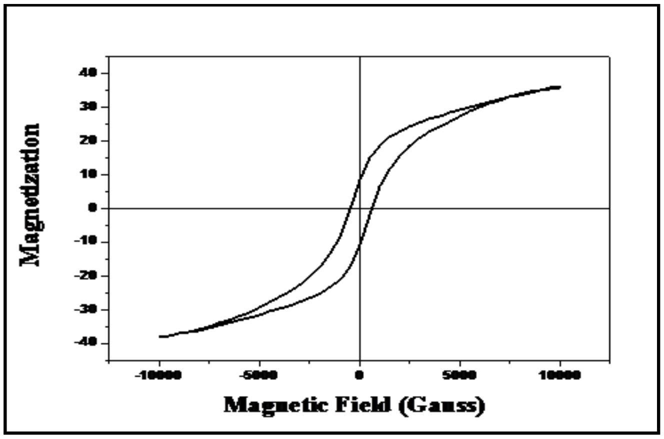


Figure 3. VSM analysis of $CoFe_2O_4$ Nano thin films (Hysteresis loop).

Effect of pH: The photocatalytic degradation of Congo red dye was studied at different pH values as it is an important parameter for reaction taking place on the particular surface. The role of pH in photocatalytic degradation of dye was studied in the pH range 0-11 at dye concentration 30 mg L^{-1}. It is observed that the rate of photocatalytic degradation enhanced with an increase in pH up to 7 as shown in the (Fig-4). As the pH increases, dye surface becomes basic. In this basic form it forms a bond with $CoFe_2O_4$ thin film. When the pH increases onwards 7 the repulsion of the dye molecules by $CoFe_2O_4$ surface would result in reduction in efficiency of degradation of CR.

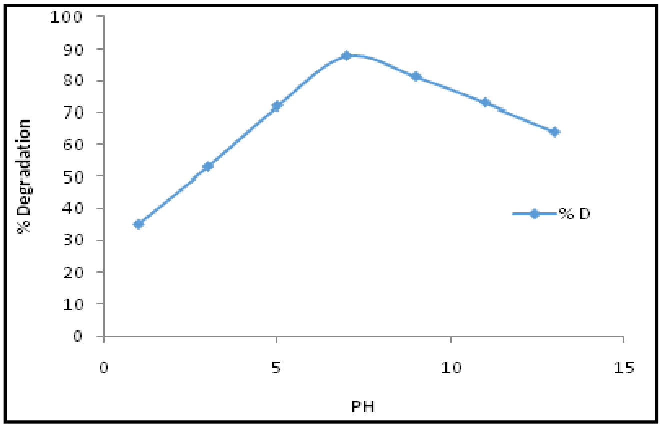


Figure 4. Effect of pH on removal of Congo red dye by $CoFe_2O_4$ thin film.

Effect of initial dye concentration: The rate of degradation of Congo red dye was studied by varying the dye concentration from 10 to 100 mg L^{-1} because of fixed catalyst concentration active sites remains the same. With the increase of the initial Congo red concentrations, the Congo red molecules get accumulated on the surface of $CoFe_2O_4$ thin film. However, quenching between these excited Congo red molecules irradiated by visible light will takes place. The quenching probability could also increase with the increase of the initial Congo red concentrations. Consequently, the photocatalytic efficiency of the Congo red dye solution was decreased with the increase of the initial Congo red concentrations is shown in the (Fig 5).

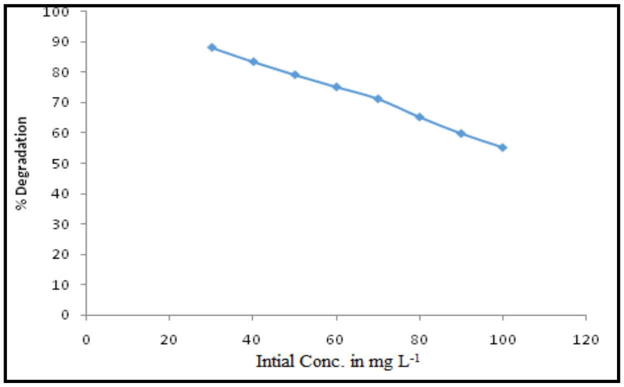


Figure 5. Effect of initial concentration of Congo red dye on % degradation at pH 7.

Effect of contact time: The effect of contact time for the photocatalytic degradation of CR dye by $CoFe_2O_4$ thin film as shown in the (Fig 6).The dye is slowly degraded in first 30 min and then degradation rate increases rapidly and reaches equilibrium in about 130 min. The rate of degradation of dye is initially slow because the surface of $CoFe_2O_4$ thin film is not efficiently activated, as the thin film surface get activated rate of degradation of dye increases rapidly.

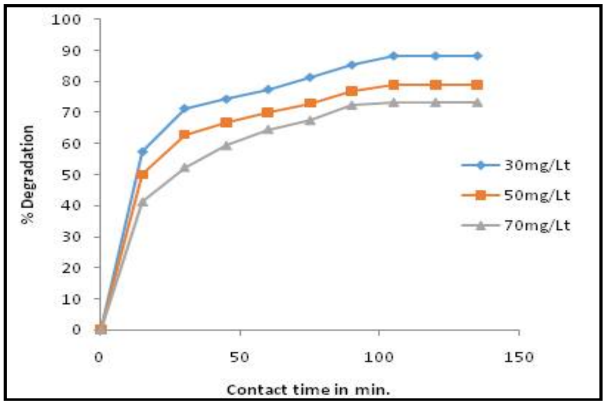


Figure 6. Effect of contact time on % degradation of Congo red at pH 7.

APPLICATION

The results indicate that this magnetic nano thin film has great potentials to be used as water purification media, where the potential of this material can be further modified to increase its degradation capacity towards targeted compounds. So this magnetic nano thin film can be successfully applied for the removal carcinogenic Congo red dye from an aqueous solution.

CONCLUSIONS

Azo dyes are one of the major contaminants present in industrial wastewater. It enters the environment when released through waste water and exerts detrimental effects on flora and fauna. The proposed nanomaterial found to be useful for the waste water purification. The prepared magnetic nano thin film was successfully applied for the removal carcinogenic Congo red dye from an aqueous solution. This magnetic nano thin film has great potentials to be used as water purification media, where the potential of this material can be further modified to increase its degradation capacity towards targeted compounds.

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Memorandum of Understanding for Academic Cooperation

between

METs Institute of Engineering, Bhujbal knowledge city, Nasik

and

NTVS's G. T. Patil Arts Commerce and Science College, Nandurbar

In accordance with a desire to take the guidance of experts, the **METs Institute of Engineering, Bhujbal knowledge city,** Nasik, has entered into this formal statement of collaboration in the form of Linkage with **NTVS's G. T. Patil Arts Commerce and Science College, Nandurbar** for encouraging students in getting a varied training through programs to be suggested by both the above collaborators.

The institution has agreed to explore and utilize the guidance and cooperation of **METs Institute of Engineering, Bhujbal knowledge city,** Nasik, and **NTVS's G. T. Patil Arts Commerce and Science College, Nandurbar:**

1. To enhance employability skills through Curriculum and Teaching Practices and discuss ways in which courses could promote scientific and technical knowledge among our students.
2. Collaborating with **METs Institute of Engineering, Bhujbal knowledge city,** Nasik, and **NTVS's G. T. Patil Arts Commerce and Science College, Nandurbar** to engage in an online exchange of ideas and pedagogic materials, be the basis for professional development activities such as Seminars, Workshops and Resource persons for our faculty.
3. Jointly propose and engage in research or training programs sponsored by funding agencies, and invite each other's faculty to participate therein.

It is understood that the details of joint activities/conditions for utilization of results achieved, arrangements for specific visits, exchange, and all other forms of cooperation will be handled on mutually agreeable terms for each specific case.

This MoU will take effect from the date it is signed by representatives of the two institutions. It will remain valid for five years and may be continued thereafter after suitable review and agreement.

Place:

Date: December, 2020

(Prof. Dr. V. S. Shrivastava)
PRINCIPAL
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Nandurbar-425412

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Science College, Nandurbar

J Mater Sci: Mater Electron **(2023)34:875**

Electrodeposition of Bi_2Te_3 thin films for thermoelectric applications: effect of electrolyte pH

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ABSTRACT

Modern materials like Bi_2Te_3 nanostructures are one of the most promising thermoelectric materials since they show a high value of the thermoelectric figure of merit. This paper reports the effect of electrolyte pH (in a low pH range starting from 0.25 to 1.50) on the structural, electrochemical, and thermoelectric properties of the electrodeposited Bi_2Te_3 films. Two of the samples showed significantly high values of Seebeck coefficient (49.28 μV/T and 45.26 μV/T, respectively), which are comparable to the Si (42 μV/T), SiC nanowires (40 μV/T), and Ge (47 μV/T) thermoelectric materials. Also, the observed crystallinity and electrochemical behavior are in agreement with the thermoelectric results for electrodeposited Bi_2Te_3 films. In nutshell, a lower range of pH of electrolytes has been found to be a significant control parameter in the present study. Such Plausible tailoring of properties would be helpful for the systematic study of complex and multi-composite materials for various applications.

1 Introduction

There are many thermoelectric materials being studied in the form of thin films. Materials like Bismuth Chalcogenides [1], Lead tellurides [2, 3], Inorganic Clathrates [4, 5], Mg-B^{IV} compounds [6, 7], Homologous oxides [8, 9], Half-Heusler alloys [10, 11] etc.

Among these materials, in the current thread of research, Bi_2Te_3 has been studied extensively. This is due to its high value of thermoelectric figure of merit at room temperature. In addition, out of many methods of synthesis, electrodeposition method has been explored by the researchers. Electrodeposited Bi_2Te_3 nanowire arrays (12–33 μV/K), pulse electrodeposited Bi_2Te_3 thin films (− 65 μV/K), and *n*-type Bi_2Te_3 films (− 51.6 μV/K) had shown Seebeck coefficient ranging from 12 to 65 μV/K [12–14].

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Electrodeposited thin films exhibit excellent thermoelectric properties as a function of reaction parameters [15–21]. In addition, the deposition rate of various phases followed by crystallite sizes can be controlled via electrodeposition parameters. And hence, this method is suitable for depositing thin films for the purpose of thermoelectric applications.

Theoretically, a material has better thermoelectric properties if electrical conductivity of the material is high and thermal conductivity of the material is low. A conductor or a semiconductor material shows thermal conductivity on account of two major phenomena viz. transport of heat through charge carries and transport of kinetic energy through particle like behavior of lattice vibrations known as phonons. Transport of charge carriers contributes to both thermal and electrical conductivity. Thus, higher electrical conductivity by virtue of charge carrier transport also increases the thermal conductivity by this route. However, the amount of heat transported through phonons is decided by the crystal structure and crystallite size in case of crystalline solids [22, 23]. Thus, for a thermoelectric material, we need to optimize the crystallite size for optimal electric and thermal conductivities. Many studies have been reported for the deposition of Bi_2Te_3 films. However, the tailoring of the structural, electrochemical, and thermoelectric properties as a function of lower range of pH has not been explored in detail. Thus, it is indeed necessary to investigate such dependence of different properties over a reaction parameter(s). And, it may be helpful, since nowadays even more complex and multi-composite materials (like perovskite) are being studied not only for thermoelectric but also for other properties like semiconducting, photoelectric, and supercapacitive actions.

The purpose of setting the parameters is to achieve thermodynamically optimal conditions for electrochemical deposition of ions on to the substrate as well as nucleation and growth of material in the electrolyte. For this purpose, under potential deposition method was used to ensure a uniform and thin deposition of the material. The stainless-steel plates were chosen to be the deposition substrate. According to literature review, mutually induced co-deposition of Bi^{3+} and Te^{2+} ions happens if correct electrochemical parameters are set [15, 18]. The ions will be deposited together at a potential more positive than both the deposition potentials of individual ions. It is also required that formation of the said ions must occur when the precursors are dissolved into the solvent. With these conditions in place, optimized deposition potential was explored earlier and found out to be − 400 mV/SCE at room temperature [20]. To optimize thermal and electrical properties as function of crystallinity through exploring the lower range of pH for electrodeposition of Bi_2Te_3 thin film is the aim of present study.

In this article, we report the properties of 6 films that were deposited at the optimum deposition potential of − 400 mV/SCE with pH varying from 0.25 to 1.5 in the interval of 0.25 and designated as P1 to P6, respectively. The range for pH parameter is selected as per the Pourbaix diagram for electrodeposition carried out with the route as stated below [15]

$$TeO_2 + H^+ \rightarrow HTeO_2^+; (0.37 < pH < 0.07) \tag{1}$$

$$HTeO_2^+ + H^+ \rightarrow Te^{+4} + H_2O \tag{2}$$

$$Bi_2O_3 + 4H^+ \rightarrow 2BiOH^{+2} + H_2O; at pH < 0.047 \tag{3}$$

$$BiOH^{+2} + H^+ \rightarrow Bi^{+3} + H_2O \tag{4}$$

$$3Te^{+4} + 2Bi^{+3} \rightarrow Bi_2Te_3 + 18e^- \tag{5}$$

For Eqs. 1–4, the rate of the reaction will be decided by the H^+ ion concentration, i.e., pH of the solution. Since pH of the electrolytes decides the deposition rates of Bi and Te, the quality of co-deposited product is in turn impacted. Quality parameters include purity (relative amounts of Bi_2Te_3, Te, Bi, and other compounds) and crystallinity (phases and crystallite size). These parameters affect the electrical and thermal properties of the deposited material which is to be used for thermoelectric applications.

2 Experimental procedures

In the present synthesis, solutions of A.R. grade bismuth nitrate ($Bi_2(NO_3)_3.5H_2O$) and tellurium dioxide (TeO_2) were prepared in nitric acid (HNO_3), respectively, in two different beakers, wherein $Bi_2(NO_3)_3.5H_2O$ acts as a precursor of Bi^{3+} and TeO_2, that of Te^{2-} explained in the following steps as shown in Fig. 1 [15, 18, 20].

First, the bath of 7.5 mM Bi^{3+} was prepared by adding 0.90 gm of bismuth nitrate in 250 ml of 1 M nitric acid and kept for 15 min until a uniform mixture was formed. Second, 0.1 M ethylene diamine tetra acetic acid (EDTA), a complexing agent, was then prepared in 100 ml double distilled water. Third, 3 ml of 0.1 M EDTA then added to the first bath containing bismuth source to obtain Bi^{3+} EDTA complex. Fourth, 10 mM solution was prepared in 1 M (250 ml) of nitric acid under constant stirring at 80 °C temperature for 30 min. Fifth, 13.5 ml of Te^{2-} precursor solution was slowly introduced into the 16.5 ml that of Bi^{3+} EDTA complex precursor solution under constant stirring. The pH of prepared electrolyte was varied from 0.25 to 1.5 with increase of 0.25 using liquor ammonia. The reaction is considered to be based on slow release of Bi^{3+} and Te^{2+} ions in the presence of EDTA, which helps for obtaining the soluble species of the Bi^{3+} in acidic medium during the synthesis process [4]. The electrodeposition was carried out for different pH [P1–P6] of electrolyte mixture of 7.5 mM Bi^{3+} and 10 mM TeO_2 at − 400 mV/SCE at room temperature for the deposition time of 40 min and named as P1–P6, respectively. The flowchart in Fig. 1 shows the stepwise process involved in the electrodeposition of Bi_2Te_3 thin films as function of pH [15, 18, 20].

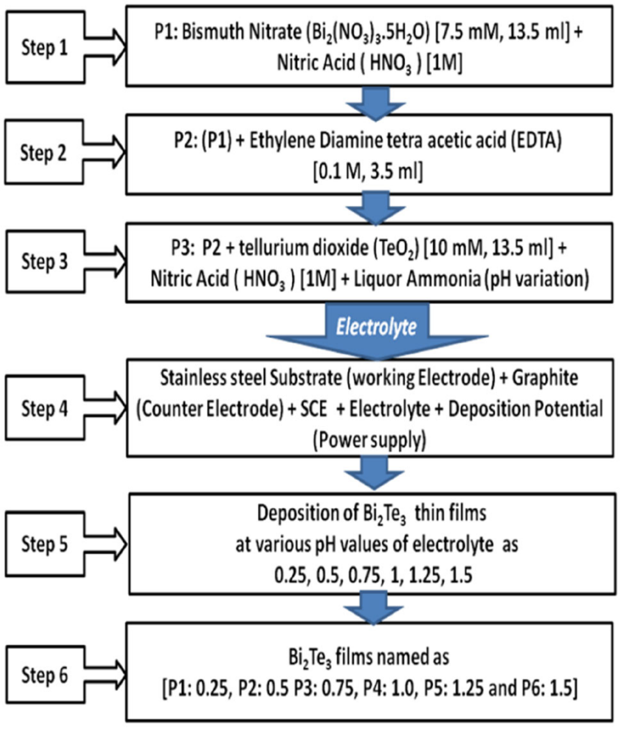

Fig. 1 Stepwise process involved in the electrodeposition of Bi_2Te_3 thin film of samples (P1–P6)

3 Results and discussion

The prepared films were characterized to determine the properties viz. elemental composition, crystal structure, phase, crystallite size, morphology, thickness, and thermoelectric properties (Seebeck Coefficient, Power Factor and Figure of merit). These results are presented and discussed below.

Cyclic voltammetry (CV) analysis for precursors and their mixture at various pH and concentration was carried out using Potentiostat Interface model 1000 (IFC100004015, Garmry). Thicknesses of the all the deposited films were measured with weighing balance made by Shimadzu (AUX220) having least count of 10 mg. Structural analysis and phase detection of the Bi_2Te_3 crystals in the electrodeposited films were carried out with the help of Panalytical Xpert PRO X-ray diffractometer (XRD) with Cu Kα radiation (λ = 1.5405 A°). Surface morphology and compositional analysis were carried out using a scanning electron microscope (JEOL-JSM 6360) (SEM) with energy-dispersive X-ray spectroscopy (EDXS) Hitachi High (S 4800 Type II) with acceleration voltage at 20 kV. Electronic properties were studied using Hall probe method ECOPIA hall effect measurement system (HMS-3000). Seebeck coefficient measurement was carried out with the laboratory made setup (Two K type thermocouples, Rishabh multimeter (Multi 14S), HTC (DT302) Thermometer). Thermal conductivity was measured with the Nanoflash (LFA 447) Netzsch instrument. The phase analysis of samples using XRD patterns has been made using Xpert Highscore package with Reference Intensity Ratio (RIR) method (more confident).

3.1 Cyclic voltammetry

Cyclic voltammetry curves were recorded during deposition process and are shown in Fig. 2 for the films P1–P6 (7.5 mM Bi^{3+}, 10 mM TeO^{2+}, and 0.1 M EDTA). The curves show distinct oxidation and reduction peaks within the potential range of − 400 mV/SCE to 700 mV/SCE. For P1 film, we see an oxidation peak at 432.0 mV and reduction peaks at − 343.9 mV and − 250 mV. The reduction peaks indicate the deposition of Te ions through two different modes [15]. Single oxidation peak for P1, P2, and P3 CV curves indicates that deposited material indeed is Bi_2Te_3. However, in case of P1 and P2, the presence of Nucleation loop indicates irreversible Te–

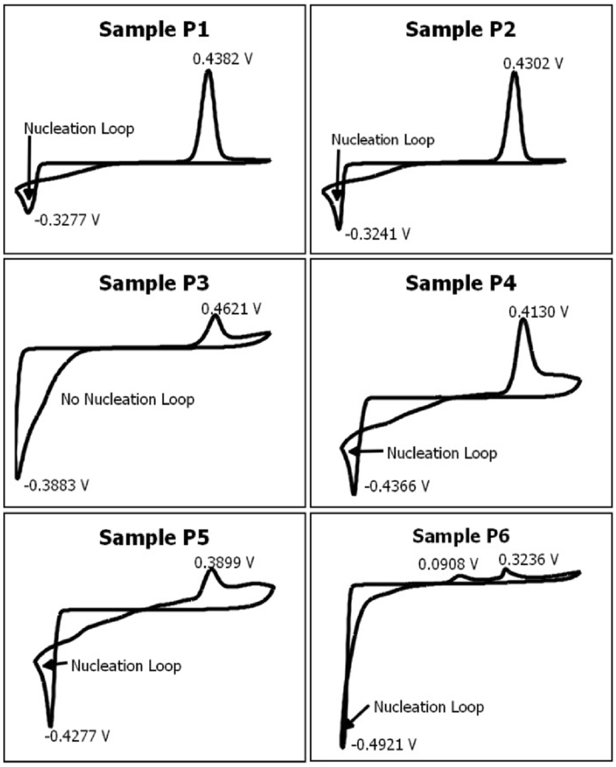

Fig. 2 Cyclic voltammograms Bi_2Te_3 with different pH values from (P1–P6)

Te deposition [15], while in case of P3, large reduction peak indicates dominant but reversible Te–Te deposition. While in case of P4, P5, and P6 films, there is additional small oxidation peak after the Bi oxidation peak. This may correspond to decomposition of Te or Bi atoms. In case of P4 and P5, the nucleation loop similar to that in P1 and P2 indicates irreversible Te–Te deposition. In addition to the major reduction and oxidation peaks, there are other oxidation and reduction peaks present in case of Samples P4 and P5 which again may correspond to decomposition of the deposited Bi and Te.

Another major aspect of the CV analysis is regarding movement of the oxidation and reduction peaks with the pH parameter. P2 shows dominant deposition of Bi at moderate oxidation potential of 4.302 V while P1, P3, and P4 show such deposition at higher potential and P5 and P6 at lower potential.

In case of deposition of Te by reduction, P2 shows lowest negative potential of (− 0.3241) for deposition while all other samples show reduction peaks of Te at a larger negative potential [12].

3.2 Thickness

Thicknesses of the films were measured using indirect weighting difference method. The average thicknesses of the films are plotted in Fig. 3. P2 sample shows the largest average thickness while P4 shows the smallest. This parameter indicates the rate of deposition of the material since the films are deposited within the same amount of time interval. Thickness of the material was assumed to be uniform as we are using electrochemical method for deposition.

Any parameter that is calculated here onward is intrinsic parameter. It is desirable to have thinner films so that the parameters will be better since the parameters are usually calculated per unit volume or mass.

3.3 X-ray diffraction

X-ray diffraction patterns for all the samples are shown in Fig. 4. The XRD patterns show the presence of polycrystalline structure. Signature peaks of Bi_2Te_3 around 2θ ~ 27.74°, 41.02°, 44.32°, and 50.44° corresponding to (h k l) planes (0 1 5), (1 1 0), (0 0 15), and (2 0 5) [24], respectively, are seen in all the samples. Intensities of the most prominent peak (0 1 5) can be seen to have different intensities relative to other peaks for different samples.

Further, Table 1 shows the average crystallite sizes, micro-strains, and dislocation densities for the films P1 to P6 obtained using the full width at half-maximum (FWHM) from XRD patterns.

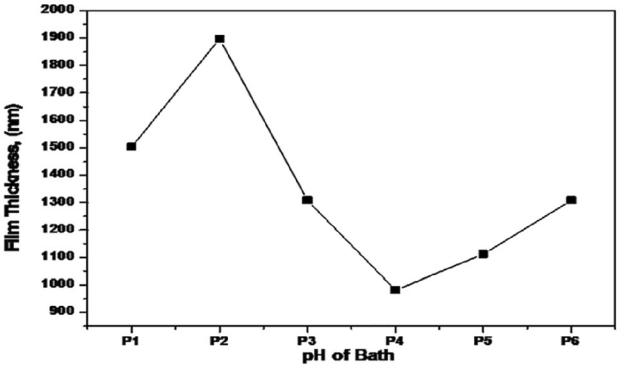

Fig. 3 Thickness variation of the samples (P1–P6) for deposition time of 40 min

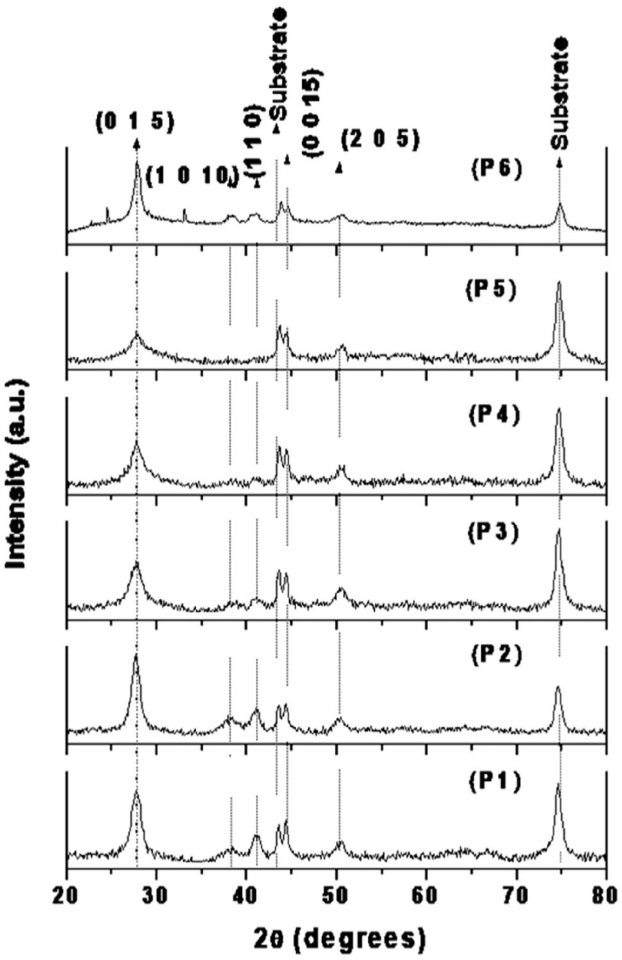

Fig. 4 X-ray diffraction patterns of samples (P1–P6)

Table 1 XRD analysis for [0 1 5] plane

#	2θ	a	β	D	ε	δ
P1	27.74	3.21	1.122	7.61	47.53	231.77
P2	27.54	3.23	1.108	7.71	46.61	171.82
P3	27.68	3.22	1.124	6.89	52.53	261.17
P4	27.72	3.21	1.565	5.46	66.30	415.94
P5	27.72	3.21	1.702	5.02	72.10	491.95
P6	27.81	3.20	0.871	9.81	36.84	128.78

sample number, 2θ Bragg's Angle in degrees, *a* lattice parameter in angstroms, β FWHM in degrees, *D* crystallite size in nanometres, ε microstrain in 10^{16} linesm^{-2} and δ dislocation density in 10^{-4}line^{-2} m^{-4}

For the analysis, Scherer's equation and standard JCPDS card No: 15-0863 [24] for Bi_2Te_3 were used.

Scherer's equation is given below:

$$\tau = \frac{K\lambda}{\beta \cos(\theta)}$$

where, τ is the mean crystalline domains size, K is the shape factor, λ is the X-ray wavelength, β is the FWHM, and θ is the Bragg angle.

Samples P1, P2, and P6 show narrower and larger (0 1 5) peak while P3, P4, and P5 show wider and smaller (0 1 5) peaks. Widening of the peaks is due to small crystallite size (in nanometres) as well as due to induced microstrain in the films. Larger intensities of the material compared to peaks of the substrate indicate larger phase percentage. (1 0 10) and (1 1 0) peaks are present prominently in only P1, P2, and P3 samples. (0 0 15) peak is present in all the samples but for P6, the peak is smaller as compared to other samples. Note that the samples P2 and P6 show all the peaks and larger (0 1 5) peak as compared to the substrate peak. From this analysis, we conclude that P2 and P6 must have significant amount of Bi_2Te_3 crystallites. This is further confirmed by phase analysis performed using RIR method from XRD data as indicated in Fig. 5.

The crystallite size analysis indicates that P6 followed by P2 has the largest crystallite size and thus the lowest microstrain.

3.4 Elemental analysis

Elemental analysis performed using EDAX is shown in Table 2. Samples P2, P3, and P4 are relatively closer to the actual stoichiometric ratio of 0.67 for the compound. However, it has been proved before that this material can exist in same phase with different

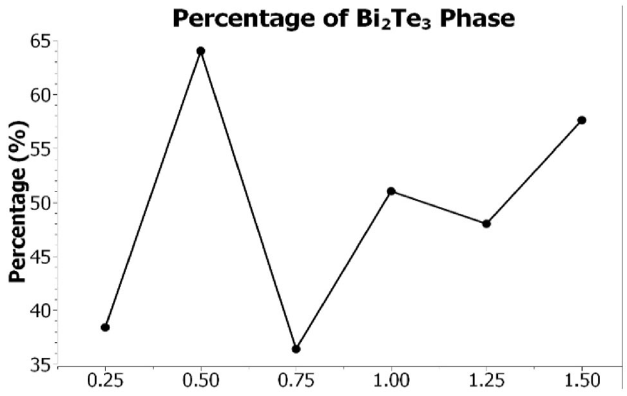

Fig. 5 Bi_2Te_3 Phase amount for the samples (P1–P6) using XRD data

Table 2 Elemental analysis for samples (P1–P6)

Sample	Bi%	Te%	Bi/Te
P1	54.28	45.72	1.19
P2	49.31	50.69	0.97
P3	46.43	53.57	0.87
P4	48.94	51.06	0.96
P5	57.11	42.84	1.33
P6	57.90	42.10	1.38

stoichiometric ratios [15]. Samples P1, P5, and P6 are quite Bi rich as compared to other 3.

3.5 Scanning electron microscopy

Figure 6 shows the SEM images morphology of the samples. All samples exhibit dendritic masses fused together to various degrees (refer to high resolution figures located at the insets of the SEM images). SEM images show a fused mass of dendrites for P1 sample, relatively separated dendritic masses in the form of aggregated balls for P2. While P3 shows morphology similar to P2 but for P2, the balls have more clear boundaries than P3. The SEM image for P3 also shows two different areas, light and dark, which may be interpreted as follows. Dark area refers to a flatter morphology with less dense mass, while light areas refer to balls shaped areas. P4 shows morphology with dendrites forming a continuous mass similar to P1 but with larger voids which are in the case of this particular snap is all oriented along same direction. P5 and P6 both again show aggregated balls type morphology. But P6 has the dendritic structures more separated than P5.

Morphology of the structure is an important parameter since thermal as well as electrical conductivities depend on the morphology. One can conclude that, more fused dendritic structures results in to the good thermal conductivity. Such large values of conductivity are detrimental to the thermoelectric effect as per the obtained figure of merit (ZT) in the present work [25–27]. Thus, we expect P2 and P6 to perform better as a thermoelectric material provided they show good electrical conductivity.

3.6 Thermal conductivity

Thermal conductivities of the samples were measured and are plotted in the Fig. 7.

High thermal conductivity of P3 brings down the performance of the film, while P2 has relatively high but still low enough thermal conductivity in addition to the co-deposition-favored crystal structure which is favorable for better thermoelectric performance. For all other samples, the thermal conductivity is very low. If the electrical conductivities of these samples are high enough the samples will perform better as thermoelectric materials [22, 23].

3.7 Four probe

The electrical conductivities of the samples shown in Fig. 8 are measured using four probe methods. Highest conductivity was shown by the P3 sample while others show significantly lower conductivities. P2 exhibits second best value for conductivity. However, as stated, earlier to large value of thermal conductivity may become detrimental for a thermoelectric material. We may expect P2 to be one of the best thermoelectric materials from all the samples since it shows the combination of favored co-deposition, moderate thermal conductivity, as well as moderate electric conductivity.

Low conductivity despite large crystallite size of samples P1, P5, and P6 may be due to the Bi richness which was discussed in elemental analysis section.

Which means though these samples show larger crystallites, the crystallites may be surrounded by Be-rich phases. Hence, such deposition shows lower conductivity despite of larger crystallite size, whereas samples P2 and P3 show large conductivity despite smaller crystallite size. In short, not only the amount of crystal boundaries but also the ease of conduction of charge carriers across a boundary will also affect the electrical and thermal conductivity.

3.8 Seebeck coefficient and figure of merit

The Seebeck coefficients plotted in Fig. 9 for the samples are calculated using a laboratory made setup. The best Seebeck coefficient as shown in Fig. 9 was exhibited by P2 sample followed by P6, P1, and P3. As mentioned earlier, the reason for the best performance of P2 may be the combination of moderate electrical conductivity, low thermal conductivity, and co-deposition dominated phase. This agrees with the phase analysis discussed in XRD section.

Figure of merit is a performance indicator used to compare the performance of the materials. In this

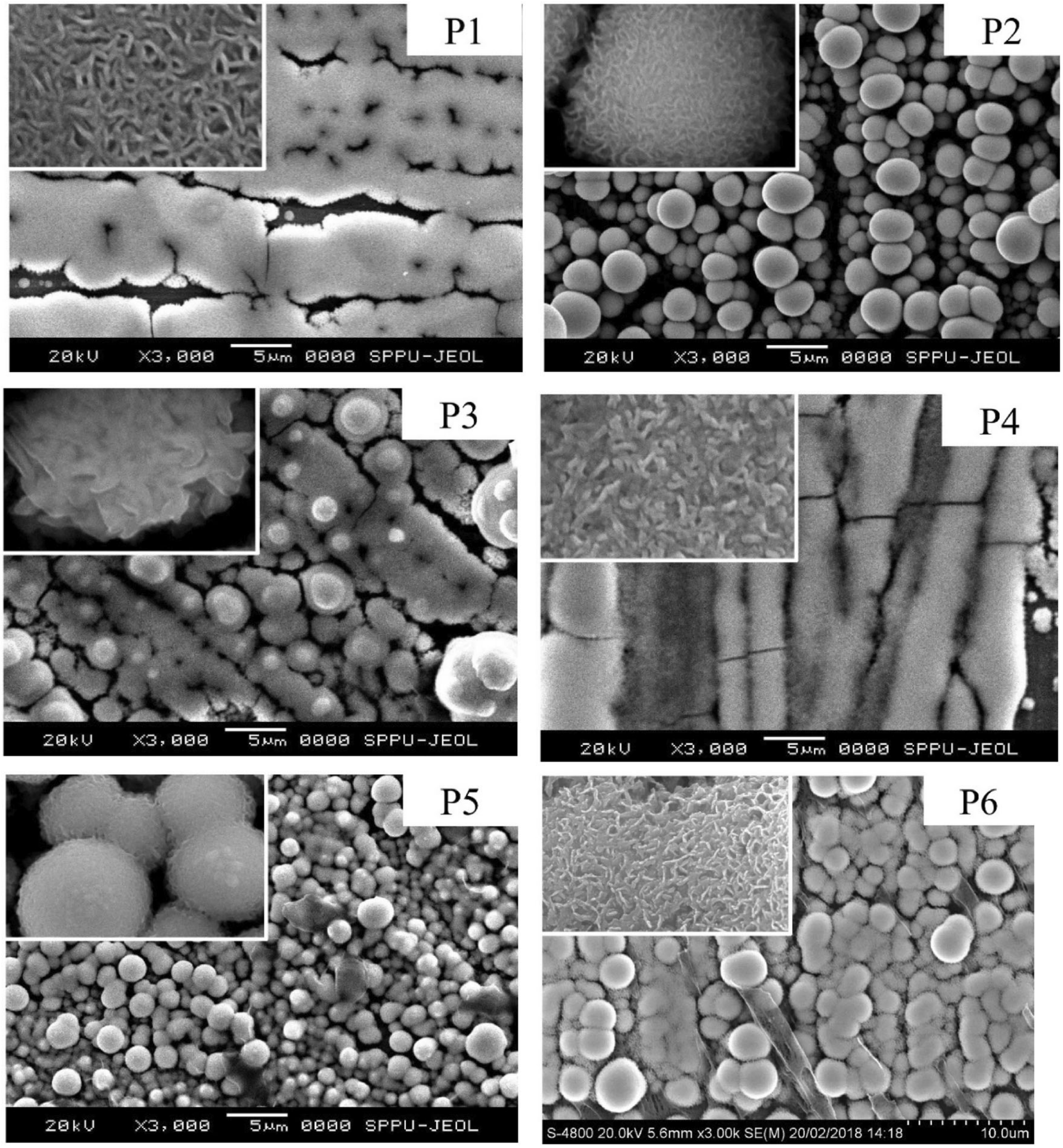

Fig. 6 Scanning Electron Images of samples (P1–P6): 3000 × main images and 6000 × (higher resolution) images in inset

case, figure of merit to measure thermoelectric performance of a material is given by [25, 26, 28]

$$ZT = \frac{\sigma S^2}{\kappa} T$$

where σ is electrical conductivity, S is Seebeck coefficient, κ is the thermal conductivity, and T is the absolute temperature.

Hence, to achieve better thermoelectric properties, the material must have high electrical conductivity, Seebeck coefficient, and low thermal conductivity [15, 25, 28, 29].

Thermoelectric figure of merits for samples (P1–P6) are plotted in Fig. 10 and are calculated using the electrical conductivities, thermal conductivities, and Seebeck coefficient of the samples.

Taking into account all electrical conductivity (large for P3 and moderate for P2), Seebeck coefficient (large for P2 and moderate for P1, P3, and P6), and thermal conductivity (large for P3 and moderate for P3 while others have low thermal conductivities), P2 performs as the best thermoelectric material followed by P6, P3, P4-P5, and P1 as per the figure of merit (ZT).

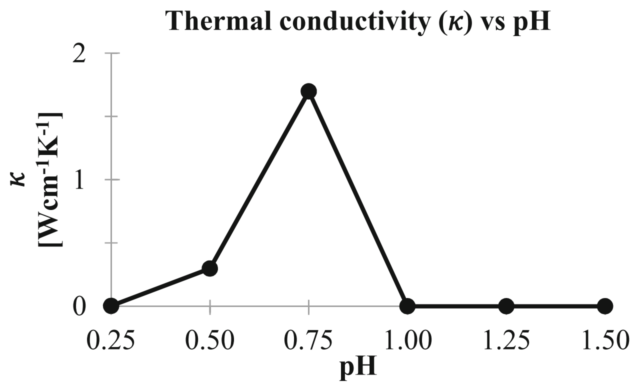

Fig. 7 Variation of thermal conductivity with pH for samples (P1–P6)

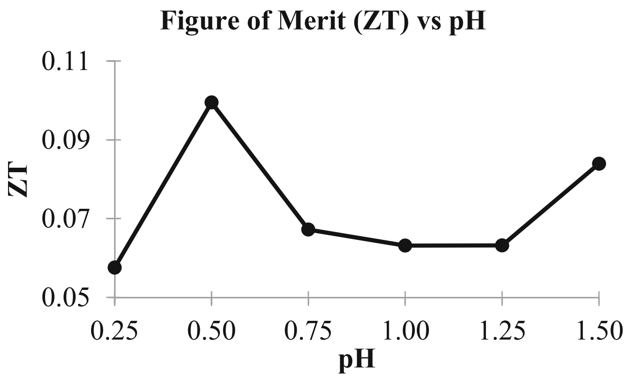

Fig. 10 Variation of figure of merit with pH for samples (P1–P6)

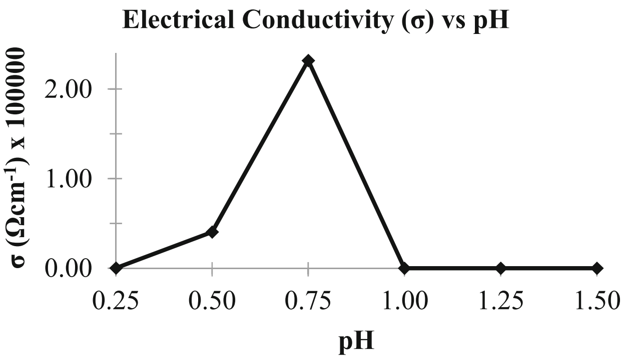

Fig. 8 Variation of electrical conductivity with pH for samples (P1–P6)

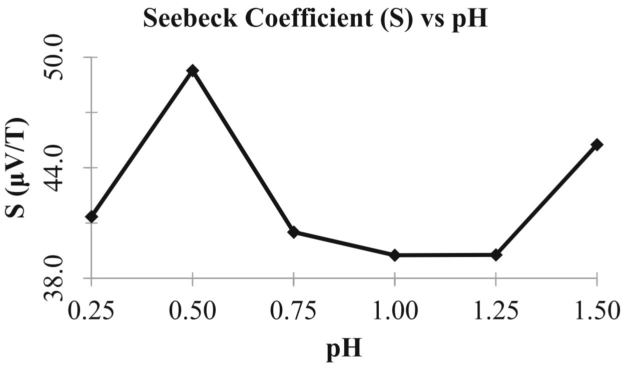

Fig. 9 Variation of Seebeck coefficient with pH for samples (P1–P6)

4 Conclusion

The paper reports successful electrodeposition of Bi_2Te_3 films for thermoelectric applications using lower pH as a control parameter. XRD and CV spectra revealed that pH has significant control over the rate of all redox reactions that are possible in given electrolyte. Hence, pH in turn controls the rate of deposition of various phases of the substance on to the substrate. Thus, variation of the pH causes variation of thermal and electrical conductivities that in turn vary the thermoelectric properties of the deposited material. This is evident from the CV and structural results that complement the thermoelectric observations.

Sample P2 found to yield better Bi_2Te_3 as a thermoelectric material (S = 49.28 μV/T, ZT = 0.099) than the Si (∼ 42 μV/T) and Ge (∼ 47 μV/T) thermoelectric materials. This performance is exhibited on account of moderate electrical conductivity and low thermal conductivity due to optimal crystallite size and phase amount. This suggests that optimization of other reaction parameters in combination with pH would open an interesting way out to study complex or multi-composite materials for various applications.

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Author contributions

All authors contributed to the study conception and design. Material preparation, data collection, and analysis were performed by VSK and ANK. Phase amount analysis from XRD was performed by MK[5]. The first draft of the manuscript was written by VVL and all authors commented on the previous versions of the manuscript. All authors read and approved the final manuscript.

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Data availability

Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

Declarations

Competing interest The authors have no relevant financial or non-financial interests to disclose.

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RESEARCH COLLABORATION

This **RESEARCH COLLABORATION** is entered into, on this date 30 /09/2019.

BETWEEN

NTVS's G. T. Patil Arts, Commerce and Science College, Nandurbar-(425412) represented herein by Principal, Prof. V. S. Shrivastava (hereinafter, referred as **'First Party'**, include its successors – in-office, administrators and assigns).

AND

Bhusawal Arts, Science and P.O. Nahata Commerce College Bhusawal-425201, represented herein by Principal, Prof. Minakshi V. Waykole (hereinafter, referred as **'Second Party'**, include its successors – in-office, administrators and assigns).

(First Party and Second Party are hereinafter jointly referred to as 'Parties' and individually as 'Party')

NOW THEREFORE, IN CONSIDERATION OF THE MUTUAL PROMISES SET FORTH IN THIS MoU, THE PARTIES HERETO AGREE AS FOLLOWS:

- **Project-Based Learning**: First Party shall design project-based activities especially for Science, Technology, Engineering and Mathematics (STEM) subjects for students of Second Party helping them excel in these subjects.
- **Training**: First Party shall design modules for training on recent technologies and share knowledge with teachers and students of Second Party.
- **Career Counseling**: First Party shall conduct exclusive sessions with students of Second Party on futuristic careers in the fields of Science & Engineering, Commerce & Management, Pharmacy, etc.
- **Student Connect**: Second Party shall share student details with First Party for one-to-one interaction and guidance on projects, models, skill development, career enhancement etc.
- **College Tour**: Get students of Second Party to experience a guided tour to campus, colleges, classrooms, laboratories, libraries, etc. of First Party.

- **Newsletters**: Students of Second Party shall have access to newsletters of First Party.
- **Events**: Students of Second Party will be regularly invited to be part of knowledge-based events and activities of First Party.
- **Resource Sharing**: Teachers and Students of Second Party will have access to online repositories of First Party for educational purpose.
- **Partner**: Parties may mention as Partner on their website.
- **Alumni Connect**: First Party shall help to connect Alumni of both Parties.
- **Validity**: This Collaboration shall be valid for 5 years from the September 2019 and each party shall be at full liberty to terminate the collaboration with mutual consent.
- **Free of Cost**: The services herein are free of cost for education purpose.

For
Bhusawal Arts, Science and P.O. Nahata Commerce College Bhusawal-425201

Signature:

PRINCIPAL
Bhusawal Arts,Science and P.O.Nahata
Commerce College, Bhusawal

Name: Prof. Minakshi V. Waykole
Designation: Principal

Date:30/09/2019

Seal:

For
NTVS's G. T. Patil Arts, Commerce and Science College, Nandurbar-425412

(Prof. Dr. V. S. Shrivastava)
Principal
PRINCIPAL
G.T.Patil Arts,Commerce &
Science College
NANDURBAR - 425 412 (M.S.)

Name: Prof. V. S. Shrivastava
Designation: Principal

Date:30/09/2019

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Center Code No.: 052

Junior College Index No.
13.12.002

Collaboration/Linkage Certificate

To whomsoever it may be concern

This is to certify that **Dr. Manohar Rajendra Patil** Department of Chemistry NTVS's G.T. Patil Arts, Commerce and Science College; Nandurbar-425412 has research collaboration (since 2017) with **Karmveer Abasaheb Alias N.M. Sonawane Arts, Commerce and Science College, Satana (Maharashtra)** for sharing the research ideas, exchange of reprints of our research papers and for the sample characterizations. We have jointly worked on research topics related to the application of nanoparticles and have published the research work in reputed international journals.

We have further extended this linkage with both the Chemistry departments to review the curriculum, teaching practices and discuss ways in which courses could be revised to promote scientific knowledge among the students.

Place: Satana

Date: 20/01/2022

Yours Sincerely

SATANA
423301
NASHIK

Principal
Karm.Abasaheb Alias N.M.Sonawane
Arts, Commerce & Science College
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"National Education Policy 2020 with Special Reference to Research and Development"
15th & 16th February, 2023

CERTIFICATE

This is to certify that, Mr./Miss./Prof./Dr. Patil Manohar Rajendra of G.T.P College Nandurbar College / Institute has worked as Resource Person / Chaires a Session / Participated / [✓ Presented a Paper] entitled Educational Policies of India : Past present and future In Oral / Poster Session in the National Seminar on **"National Education Policy 2020 with Special Reference to Research and Development"** held on 15th & 16th February, 2023.

Dr. Rajendra D. Vasait
Co-ordinator

Prin. Dr. Vijay J. Medhane
Convener

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DST FIST Identified College
Awarded "Excellent College" By North Maharashtra University, Jalgaon 2014
● GOLDEN JUBILEE YEAR 2014-15 ●
Prof. Dr. V. S. Shrivastava
Ph.D. Post. Doct. (S.America)
Principal
Office : (02564) 222293, 226534
E-mail: gtpcollege@rediffmail.com
drvinod_shrivastava@yahoo.com
Web: www.ntvsgtpcollege.org

G.T.P.C. A/No./977/

Date: 25/03/2022

Permitted
29/03/2022

The principal,
SSBT'S College of Engineering,
Bambhori, Jalgaon
Date: 25/03/2022

Subject: Allowing our students to work with Dr. Kiran S. Patil in your esteemed Institute

Respected Sir,

It gives me an immense pleasure to inform you that two of our faculties namely **Dr. Gaurav R. Gupta** from Department of Chemistry GTP College, Namdurbar and **Dr. Kiran S. Patil** from your esteemed Institute having research collaboration and I am sure this collaboration definitely uplifts the standard of their research . In this regard, I am requesting you please allow four of our P.G Student [M.Sc.II: Organic Chemistry] namely **Shubham V. Patil, Rahul A. Chavan, Rohit D. Patil** and **Avinash More** for the research with **Dr. Kiran S. Patil** at your institute. Also, we continues such collaborative research for the upliftment of the standard of the research.

Thanking You.

Yours Sincerely,

Prof. Dr. V. S. Shrivastava

PRINCIPAL
Gajmal Tulshiram Patil
College,Nandurbar

MEMORANDUM OF UNDERSTADING

This **Memorandum of Understanding** (hereinafter called as the 'MoU') is entered into, on this date 30/04/2022 (DATE).

BETWEEN

Shram Sadhana Bombay Trust's College of Engineering & Technology, Bambhori, Jalgaon-425001 (M.S.), on behalf of SSBT's Group of Institutions, represented herein by Principal, Dr. Girish Kumar Patnaik (hereinafter referred as **'First Party'**, include its successors – in-office, administrators and assigns).

AND

NTVS's G. T. Patil Arts, Commerce and Science College, Nandurbar (NAME OF SCHOOL) represented herein by Principal, Prof. V. S. Shrivastava (NAME) (hereinafter referred as **'Second Party'**, include its successors – in-office, administrators and assigns).

(First Party and Second Party are hereinafter jointly referred to as 'Parties' and individually as 'Party')

NOW THEREFORE, IN CONSIDERATION OF THE MUTUAL PROMISES SET FORTH IN THIS MoU, THE PARTIES HERETO AGREE AS FOLLOWS:

- **Project-Based Learning**: First Party shall design project-based activities especially for Science, Technology, Engineering and Mathematics (STEM) subjects for students of Second Party helping them excel in these subjects.
- **Training**: First Party shall design modules for training on recent technologies and share knowledge with teachers and students of Second Party.
- **Career Counseling**: First Party shall conduct exclusive sessions with students of Second Party on futuristic careers in the fields of Science & Engineering, Commerce & Management, Pharmacy, etc.
- **Student Connect**: Second Party shall share student details with First Party for one-to-one interaction and guidance on projects, models, skill development, career enhancement etc.

- **College Tour**: Get students of Second Party to experience a guided tour to campus, colleges, classrooms, laboratories, libraries, etc. of First Party.
- **Newsletters**: Students of Second Party shall have access to newsletters of First Party.
- **Events**: Students of Second Party will be regularly invited to be part of knowledge-based events and activities of First Party.
- **Resource Sharing**: Teachers and Students of Second Party will have access to online repositories of First Party for educational purpose.
- **Partner**: Parties may mention as Partner on their website.
- **Alumni Connect**: First Party shall help to connect Alumni of both Parties.
- **Validity**: This MOU shall be valid for 3 years from the date 30/04/2022 (DATE) and each party shall be at full liberty to terminate the collaboration with mutual consent.
- **Free of Cost**: The services herein are free of cost for education purpose.

For
SSBT's College of Engineering & Technology,
Bambhori, Jalgaon -425001(M.S.),
on behalf of SSBT's Group of Institutions

Signature:
PRINCIPAL
SSBT's College of Engineering & Technology
Bambhori,Jalgaon-425001(M.S.)
Name: Dr. Girish Kumar Patnaik

Designation: Principal

Date: 30/04/2022

Seal:

For
NTVS's G. T. Patil Arts, Commerce and
Science College, Nandurbar-425412

Signature:
PRINCIPAL
Gajmal Tulshiram Patil
College,Nandurbar
Name: Prof. V [illegible]

Designation: Principal

Date: 30|4|2022

Seal:

To
Principal
COET, Bambhori
Jalgaon

Date: 02/05/2022

Subject: Need of hostel facility to the PG students [M.Sc. II]

Dear sir,

As per above cited subject, the students of G.T Patil college Nandurbar are visiting to our college in applied science department for project related work. The MOU is done with this institute. The visit of the students is planned in between 02/05/2022 To 20/05/2022. (15/5/2022) kindly allowed them to stay at hostel on non-payment basis.

The details are as below,

College Name	Students Name	Mobile No.
G.T. Patil College Nandurbar [M.Sc. II]	1. Shubham V. Patil	9403698399
	2. Rohit. D. Patil	7768912265
	3. Rahul A. Chavan	9834707452
	4. Avinash H. More	8888927493
	5. Akshay Borse	8857032635

Kindly do the needful

2/5/2022
HOD, Applied Science
Dr. Kiran Patil.

Considering MoU signed and
college/students from Nandurbar,
single room in the hostel
please be allotted with
Rs 50/- per room per day
(Rs 10/- per person, per room, perday) charges.

R.P. [illegible]/2022

SSBTs COLLEGE OF ENGINEERING AND TECHNOLOGY HOSTEL

Receipt Voucher

Name. : G.T.Patil College Nandurbar

ID. : 28666

Dated : 02/05/2022

Particualrs	Amount	
Account		
HOSTEL GUEST CHARGES	700.00	
CASH		
On Account Of : Received from Shubham V Patil Rohit D Patil Rahul A Chavan Avinash H More and Akshay Borase against Hostel Guest Charges Rs.10 per person per room per day 14day G.T.Patil College Nandurbar		
Amounts (in words) : Rupees- Seven Hundred Only		
	₹ 700.00	

Cashier

SSBT's College of Engineering & Technology,Bambhori,Jalgaon

0 2 MAY 2022

नकद प्राप्त/CASH RECEIVED

CASHIER

Principal/Director

( )

KAVAYITRI BAHINABAI CHAUDHARI NORTH MAHARASHTRA UNIVERSITY, JALGAON

KBCNMU/11/Ph.D./Chem./Online/2022

Date : 01-12-2022

To,

Mr. PRAVIN NAMADEO MORE

Subject:- Provisional admission to Ph.D. Course in the Subject of Chemistry under the faculty of Science and Technology

Dear Student,

With reference to the above subject, it is to inform you that, based on your qualification/exemption for the PET 2021 examination, and allotment of guide, you are provisionally registered for Ph.D. course from the date as mentioned below. Your Ph.D. registration will be confirmed on successful completion of Pre-Ph.D. course work and presentation of research outline before RRC within a stipulated period as per rules (Regarding the programme of conduct of the course work, you are requested to visit University's website **https://www.nmu.ac.in**). The particulars of your admission are as under:-

Sr. No.	Particulars	
1.	Name of Guide	Dr. Gupta Gaurav Ramesh
2.	Name of Co-guide	
3.	Place of Research Work	Laboratory / Research Center recognized by KBCNMU, Jalgaon
4.	Provisional date of Registration	Guide Allocation Meeting 14-10-2022
5.	Registration No.	KBCNMU/11/Ph.D./Chem./932/2020
6.	Application No.	PHD-2021-SXAGZ6 [Exemption] .
7.	Fees Payment Details	Paid Rs. 22750.00 on 18-12-2022 12:31:06

Your attention is also invited to the following points regarding Ph.D. course admission :-

1. You will have to abide by the rules made by the University from time to time as per provision under Section 60 of the Maharashtra Public Universities Act, 2016 and the rules for the admission for Degree of Doctor of Philosophy (Ph.D.) as per the UGC (Minimum standards and procedure for awards of Ph.D. degree) Regulation 2009 and 2016 and revised Ph.D. rules from time to time.
2. You are requested to pay the following fees as prescribed by the University Authorities from time to time within one month from the date of issue of this letter. **The yearly fees will be charged every year from the date of registration.**

A) To be deposited in the University

Sr. No.	Head	First Year (Fee) Rs.		Subsequent Years Fee Rs.	
		For Science & Technology	Other than Science & Technology	For Science & Technology	Other than Science & Technology
1.	Provisional Registration Fees	1000/-	1000/-	0	0

AGREEMENT

THIS AGREEMENT is made on this 21st day of September 2022.

BETWEEN

UPL Limited a Company incorporated under the Companies Act of 1956 and having its Registered Office at 3-11, GIDC, Vapi -396 195, Gujarat and Corporate Office at UPL House, 610/B2, Bandra Village, Off Western Express Highway, Bandra (East), Mumbai 400 051 (hereinafter referred to 'the Company') of the ONE PART

AND

Mr. **Pravin Namadeo More** residing at **D-1, UPL colony-1 , Near Manav mandir, GIDC , Ankleshwar Gujrat 393002** (hereinafter referred to 'the Employee') of the OTHER PART.

WHEREAS the employee had joined the Company on 2nd February 2004. His current designation is Group lead Formulations.

AND WHEREAS on the request of the employee, Company has agreed to permit the employee to pursue higher studies in Ph.D. during the tenure of the employment and the detail of such course is mentioned in Schedule 'A' hereunder.

AND WHEREAS Employee and the Company have agreed on various terms and conditions as follows:

NOW IT IS AGREED BY AND BETWEEN THE PARTIES HERETO AS FOLLOWS:

1. (a) The expression "the Company" in this Agreement shall mean and include the successors and assigns of as also any firm, person, or company subsidiary to or affiliated with, or having a controlling interest in, the Company.

   (b) The expression "he", "his" or other words imparting masculine gender shall be taken to include feminine gender, where the Employee is a female.

2. The Company has agreed to permit the employee to pursue higher studies and/or enhance the qualification as mentioned in Schedule 'A' of the employee during the tenure of his employment with the Company.

3. The employee has agreed to carry out such studies without affecting his regular working with the Company.

4. The employee is permitted to utilize the Laboratory, and/or the library and/or other facilities as may be made available to the employee from time to time with prior permission from HOD/Unit Head. However, in case of any damages to the property of the Company, it will be reimbursed by the employee.

5. The employee has agreed to continue working with the company at least for a period of **3 years** from the date of completion of the enhancement qualification/degree/doctorate. In case the employee leaves and/or cease to be an employee of the Company for any reason whatsoever, within a period of *3 years* from the date of completion of the course, the employee shall refund the entire amount paid by Company towards the program else, it will be recovered from the full and final settlement of the respective employee. In any event, the Company is at liberty to initiate any legal action/s against the employee as they deem fit and recover such monies paid by the company towards the program.

6. The employee has agreed not to resign and/or do any act which will make the company to terminate the employment of the employee with the Company.

7. The employee has agreed to pay 50% of the annual Fees each year for a period of 4 years Doctoral program.

8. Company has agreed to pay the balance 50% of the annual Fees under the UPL Philomath Doctoral Assistance Program ("program"), each year for a period of 4 years of the program.

9. During the tenure of program, if the employee leaves/ resigns voluntarily or if the employee is terminated for any reason whatsoever, the employee will have to refund the entire amount paid by the Company towards the said Doctoral program and/or it would be recovered from the full and final settlement of the respective employee.

10. During the tenure of this Doctoral program, if the institute suspends or expels the employee due to any kind of misconduct as per the Institutions internal policy, Company will have the right to terminate the employee from his/her services with immediate effect and the employee will have to refund the entire amount paid by the Company towards the said program and/or it will be recovered from the full and final settlement of the employee

11. In case the employee is unable to complete his/her Doctoral studies within the period of 4 years, employee will have to refund the entire amount paid by the Company towards the said Doctoral program. In any event, the Company is at liberty to initiate any legal action/s against the employee as they deem fit and recover such monies paid by the company towards the program

12. Employee agrees to indemnify the Company and keep it indemnified at all times against all or any costs, claims, damages or expenses incurred by the Company, or for which the Company may become liable, with respect to any intellectual property infringement claim or other claim relating to the Works or Inventions by the Employee during the course of this Agreement.

13. Employee agrees that this agreement, along with the employee's appointment letter together constitutes an entire agreement & understanding with the Company. All other terms of the Appointment letter are valid together with this Agreement and other subsequent agreement executed with the Company.

14. Employee acknowledges that in the course of studies he/she shall not share any confidential information with the institute. **Confidential Information** means any and all information in whatever form (including without limitation, in written, oral, visual or electronic form or on any magnetic or optical disk or memory and wherever located) relating to the business, customers, products, affairs and finances of the Company for the time being confidential to the Company and trade secrets including, without limitation, R&D data, technical data and know-how relating to the Business of the Company, its research, its products or any of its suppliers, customers, agents, distributors, shareholders, management or business contacts and including (but not limited to) information that the Employee creates, develops, receives or obtains in connection with his/her employment with the Company, whether or not such information is marked confidential.

15. No variation of this agreement shall be valid unless it is in writing and signed by or on behalf of each of the parties

16. This agreement stated in Clause 10 and any dispute or claim arising out of or in connection with it or its subject matter or formation (including non-contractual disputes or claims) shall be governed by and construed in accordance with the laws of India. The parties irrevocably agree that the courts of Mumbai shall have jurisdiction to settle any dispute or claim that arises out of or in connection with this agreement or its subject matter or formation.

IN WITNESS WHEREOF the parties have executed these presents the day, month and year first above written.

Signed and delivered by the)
Within named 'Company')
Namely UPL Limited)
Through its Authorised Signatory)
Rajan R. Shivsat)
In the presence of:)
1. Shiv Kumar Sharma

Signed and delivered by the)
Within named 'Employee')
Namely Pravin N. More)
In the presence of:)
Uttam Katulkar

SCHEDULE A

Name of the Doctoral Program	Institution	Probable Duration and Commencement Date	Probable Completion Date
Ph.D. in Chemical Sciences	*Affiliated college under Kavayitri Bahinabai Chaudhari North Maharashtra University Jalgaon*	*4 years from October 2022*	*October 2026*

SIGNED BEFORE ME
M. P. PATEL
B.Com., LL.B.
ADVOCATE & NOTARY
(Govt. of Guj.)

M. P. PATEL

Reg. No. 6932/22
Date 3 OCT 2022

INDIA NON JUDICIAL

Government of Gujarat

सत्यमेव जयते

MOHANBHAI B. PATEL

Rs. 100

Certificate of Stamp Duty

Certificate No.	:	**IN-GJ31540102917695U**
Certificate Issued Date	:	21-Sep-2022 12:21 PM
Account Reference	:	IMPACC (AC)/ gj13380611/ ANKLESHWAR1/ GJ-BH
Unique Doc. Reference	:	SUBIN-GJGJ1338061192590686165942U
Purchased by	:	JAGDISHBHAI PATEL
Description of Document	:	Article 5(g-a) Agreement - Construction / Development / Sale / Transfer (Imm. Property)
Description	:	AGREEMENT
Consideration Price (Rs.)	:	0 (Zero)
First Party	:	UPL LIMITED UNIT 3
Second Party	:	Not Applicable
Stamp Duty Paid By	:	UPL LIMITED UNIT 3
Stamp Duty Amount(Rs.)	:	100 (One Hundred only)

A. HARESHBHAI PATEL

IN-GJ31540102917695U

JD 0010831626

the date of completion of the course, the