

**INTERNATIONAL CONFERENCE ON CONDENSED  
MATTER PHYSICS AND MATERIALS  
(ICCMPPM 2023)**

28<sup>th</sup> February and 1<sup>st</sup> March 2023

**NATIONAL SCIENCE DAY CELEBRATION**



**BOOK OF ABSTRACTS**



**Organized by**  
Department of Physics  
Ethiraj College for Women (Autonomous)  
Chennai, Tamil Nadu, India

**In association with**  
INDIAN SCIENCE CONGRESS ASSOCIATION  
Chennai Chapter, Tamil Nadu, India

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**ETHIRAJ COLLEGE FOR WOMEN  
(AUTONOMOUS)**

No. 70, Ethiraj Salai,  
Egmore, Chennai - 600 008



**Thiru. V. M. Muralidharan**  
Chairman

24<sup>th</sup> February 2023

**FOREWORD**

I am delighted to learn that the Department of Physics of our College is organising, two-day International Conference on an extremely relevant, contemporary topic "Condensed Matter Physics and Materials" on the 28<sup>th</sup> February & 1<sup>st</sup> March, 2023 and releasing the Conference Proceedings on the same occasion.

I convey my heartiest congratulations and felicitations to Dr.A.V.Jhone Verjhula, Head, Department of Physics, and the members of the faculty for their sense of dedication & commitment and also to the students.

The Conference Proceedings, covering the state-of-the-art aspects, covering Energy & Environmental materials, Thin Films, Thin Films, Thermoelectric and many more topics, will certainly be a treasure trove for the students and research scholars.

The deliberations during the conference will, I am sure, trigger various ideas and drive the young minds to take independent inferences and motivate them to set higher "value" goals in their research pursuits ahead.

I seek the blessings of the Almighty and our revered founder Thiru.V.L. Ethiraj, to provide us the inner guidance and wish the department higher levels of achievements and approbations in all its endeavours.

Yours sincerely,



V.M. Muralidharan  
Chairman

## THE INDIAN SCIENCE CONGRESS ASSOCIATION

(Professional Body under Department of Science & Technology,  
Ministry of Science & Technology, Government of India)

### CHENNAI CHAPTER

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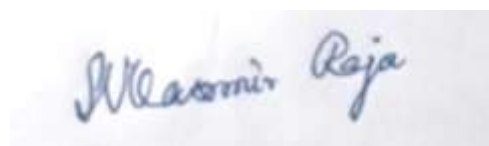
**Dr.S.V.KASMIR RAJA**

28.02.2023

Convener, ISCA Chennai Chapter

I am very much delighted to facilitate the Department of Physics of Ethiraj College for Women(Autonomous), Chennai for organizing an International Conference on “Condensed Mater Physics and Materials” on 28<sup>th</sup> February and 1<sup>st</sup> March 2023. As the Convener of the Chennai Chapter of the Indian Science Congress Association, Kolkatta, I feel proud to co-sponsor this Conference. Deeply express my hearty congratulations to The Ethiraj College founded in the year 1948 celebrating its 75 years (Platinum Jubilee) of services in Women’s education and in the Empowerment of Women.

I am sure that this two-day International conference will bring out a broad scope of Modern experimental condensed matter physics with interests ranging from macroscopic three-dimensional crystals to nanostructured solids and low-dimensional materials such as ultrathin films of metals, insulators and semiconductors, atomically-thin layers of graphene or one-dimensional quantum wires and also the studies on the properties of the large collections of atoms that compose both natural and synthetic materials. To address the problems associated with Condensed Mater Physics and Materials the Department of Physics, Ethiraj College for Women has taken a lot of initiatives to organize this conference in a fitting manner. I congratulate the organizers for their efforts and I wish them all success.



( Dr.S.V.Kasmir Raja)



## Ethiraj College For Women

(AUTONOMOUS)

**Dr. D. B. Usharani**

M.A., M.Phil., Ph.D.  
Principal i/c & Secretary i/c

### Message

I am extremely delighted to note that the Department of Physics is organising a two day International Conference on Condensed Matter Physics and Materials -ICMPPM-2023 in association with the Indian Science Congress Association Chennai Chapter, Tamil Nadu, India.

I convey my heartiest congratulations and felicitations to Dr.A.V.Jhone Verjhula Convener, Dr.S.Abhirami Co-Convener and also to the dedicated band of faculty and students of Physics Department of both Aided and Self Supporting Stream.

I thank the Indian Science Congress Association, a Premier Scientific Organisation of our country for associating with us to strengthen research in the field of Condensed Matter Physics and Materials.

I am sure the deliberations of this International conference will create new ideas, innovative results which will trigger further research.

Wishing the conference all success.

**Principal i/c & Secretary i/c**  
**ETHIRAJ COLLEGE FOR WOMEN**  
No. 70, ETHIRAJ SALAI  
CHENNAI - 600 008



**Dr. Amthul Kareem Hussain**

Former Founder and Head  
Department of Physics

### **FOREWORD**

I am overwhelmed by the warm invitation sent to me by the department of Physics for the International Conference on 28th Feb and 1st March. I have many nostalgic memories about the college I loved and the department I adored. Determination + hard work has ever been the motto of our department Young or old; rain or shine we were ever willing to go that extra mile so that we could translate our aspirations into achievements. The department of Physics is doing wonderful work under the leadership of the dynamic visionary Dr.A.V.Jhone whose watchword is EXCELLENCE and whose goal is PERFECTION. The way she inspires her colleagues and students to come out with their best is electrifying. National and international conferences and seminars have become the order of the day. On this proud moment I extend to Dr. Jhone and the department of Physics best wishes. I am confident that the program will go on rhythmically like a song.

Best Wishes to the entire team.



Dr. Amthul Kareem Hussain  
Former Founder and Head  
Department of Physics  
Ethiraj College for Women (Autonomous)  
Chennai - 600008



**UNIVERSITY OF MADRAS**  
**INSTITUTE OF DISTANCE EDUCATION**  
[Established under the Act of Incorporation XXVII  
of 1857- Madras University Act 1923]  
(State University)



**Dr. S. Aravindhan**, M.Sc., M.Phil., B.Ed., Ph.D.  
**Director**

Phone: 25613701/25613716  
Email : ide.director@gmail.com

### MESSAGE

I am honoured to felicitate the Department of Physics of the renowned Ethiraj College for Women, Chennai for organizing the International Conference on Condensed Matter Physics and Materials - ICMPPM - 2023 in association with The Indian Science Congress Association, Chennai Chapter, Tamilnadu. I am delighted to know that the Department of Physics is periodically conducting series of conferences, seminars and workshops to encourage the research drive of the stakeholders. The disciplinary area of physics being my area of specialization draws a special attraction to this conference. The theme of the conference which is related to the extensive and contemporary research area holds high relevance in the current scientific progression. The college which made a mark in the nurturing of women's education sector is now relishing its platinum jubilee. On this occasion I wish the organizing committee the very best for the splendid success of the Conference. It is a marvellous occasion, both in terms of academic quality and social indulgence. I am confident that the conference will be well-organized and conducted impeccably throughout. Let me once again congratulate the entire team who have endeavoured to make this conference into a landmark.

  
25/02/2022



**Dr. S. ARAVINDHAN**,  
M.Sc., M.Phil., B. Ed., Ph. D.,  
Professor cum Director  
Institute of Distance Education  
University of Madras  
Chennai - 600 005.



## Foreword

ICMPPM-2023 brings in lot of cheers, encouragement and motivation in the minds of faculty, researchers and young students of Ethiraj College. Achieving this in association with ISCA is a great moral and academic support. Involvement of the teams comprising College management, advisory committee and invited speakers is very impressive. As a passionate teacher and interested researcher in the field of Materials Science gives immense pleasure in participating in this international conference. This conference abstractions are compiled in such a way that the participants, budding researchers and project students get adequate knowledge in the areas of solid-state materials and its latest developments in various fields. I wholeheartedly congratulate the teams who made this conference a most susceptible to the scholars of Chennai and its surrounding. Let the legacy and glory continues in future.



**Dr C RAKKAPPAN**



### **CHIEF PATRON**

**Thiru.V.M.Muralidharan**

Chairman, Ethiraj College Trust Chennai, TamilNadu

### **PATRON**

**Dr.D.B.Usharani**

Principal i/c and Secretary i/c Ethiraj College for Women (Autonomous), Chennai, Tamil Nadu

### **ADVISORY COMMITTEE**

- Dr. Vijay Lakshmi Saxena, General President, ISCA, Kolkata, India.
- Prof. K. S. Rangappa, Former Gen. President, ISCA, Kolkata, India.
- Dr. S.V. Kasmir Raja, Convenor, ISCA, Chennai Chapter.
- Dr. C. Muthamizhchelvan, Executive. Member, ISCA & VC, SRM Inst. of Sci. & Tech., Chennai.
- Dr. M.G. Ragunathan, Executive Member, ISCA & Principal, Guru Nanak College, Chennai.
- Dr. A. Alagiriswamy, Treasurer, ISCA, Chennai Chapter & Asst.Prof., SRMIST, Chennai, India.
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- Prof. A. Stephen, University of Madras.
- Dr. Chrispin Karthick, Indian Institute of Astrophysics Bangalore.
- Prof. S. Balakumar, University of Madras.
- Prof. P. Aruna, Anna University.
- Dr. J. Madhavan, Dean of Research, Loyola College.
- Prof. Saravanan Rajendran, Universidad de Tarapaca, SERC Chile.
- Dr. Anuj Kumar, Yeungnam University, Gyeongsan, Korea.

### **CONVENER**

Dr. A. V. Jhone Verjhula

Head, Department of Physics (Aided),

### **Co-CONVENER**

Dr S Abhirami

Head, Department of Physics (SS),

**CHIEF ORGANISING SECRETARIES**

Dr. B. Uma

Dr. S. Mahalakshmi

**ORGANISING SECRETARIES**

Dr. J. Bhavani

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**TREASURER**

Dr. M. Amudha

**TECHNICAL COORDINATORS**

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Ms. A. Reshmina Tony

Mrs. A. Sakshi Joshi

Ms. R. Sravanthi

Mrs. V. Poojitha

Ms. M. Silviya

**CONFERENCE THEME:**

- Energy and Environmental materials
- Semiconductor devices
- Photonic materials
- Thin films
- Crystal growth
- Polymers, glasses, and ceramics
- Bio-materials
- Storage materials
- Thermoelectrics
- Spintronics
- Computational physics and lot more...

## **ABOUT THE COLLEGE**

Ethiraj College for Women was founded by the illustrious Barrister - at - Law, Thiru V.L. Ethiraj in 1948. The College is cherishing 75 years (Platinum Jubilee) of service in Women's education. Ethiraj College is one of the select colleges in India recognized with the award of "College with Potential for Excellence". A premier institution dedicated to the cause of women's education, was ranked number one in the Internal Quality Audit conducted by IQAC of the University of Madras in 2005. The College was re-accredited with the highest grade 'A', by NAAC in 2013 and awarded the 65th rank at the All India level by the National Institutional Ranking Frame Work, MHRD, 2021-2022. The College with 332 dedicated Teaching Faculty offers UG, PG courses, including AICTE approved MBA and MCA, Research Programmes M.Phil, Ph.D and several value added courses for around 7600 students.

## **ABOUT THE DEPARTMENT**

The Department of Physics has worked unceasingly towards its upgradation since its inception in 1948. With the introduction of post graduate degree course in 2004 and M.Phil in 2009, the Department is engaged with Research Activities in various fields of Physics by offering the Ph.D programme from 2018. National and International Conferences, Workshops and Seminars are periodically organized to promote research activities amongst the staff and students.

## **ABOUT THE CONFERENCE**

Condensed Matter Physics and Materials have a specific goal of understanding the structure, properties of all kinds of solids and liquids. It is a broad area of research in modern physics, with frequent occurrence of novel phenomena, relating to exotic properties of matter in metals, semiconductors, superconductors, magnets, insulators, and mesoscale systems.

A Two Day International Conference on Condensed Matter Physics and Materials (ICMPPM) is organized by the Department on the 28th February & 1st March 2023 in the Hybrid mode. This conference will provide a platform to academicians, teachers and young researchers to interact with distinguished scientists in the field and to know the state-of-the-art in the field of Condensed Matter Physics and Materials.

## **ABOUT THE INDIAN SCIENCE CONGRESS ASSOCIATION**

The Indian Science Congress Association was formed to advance and promote the cause of Science in India. The association is a premier scientific organization of India with headquarters at Kolkata, West Bengal. The association, started in the year 1914 in Kolkata and it meets annually in the first week of January. The major objective of the ISCA, having celebrated its Hundredth year of its inception on 2nd June 2012, is to inculcate the scientific temper among the people and to encourage young scientists to grow up steadily in the scientific direction.

**Programme Schedule – Day I**

Time (IST)	Speaker	Title of the Talk
<b>Day 1 (28.02.2023) –Hybrid Mode</b>		
09:30 – 9:45 AM	<b>Inauguration</b>	
09:45 – 10:45 AM	<b>Key Note Address</b>	
10:45 – 11:00 AM	<b>Tea Break</b>	
11:00 – 11:50 AM	Dr S C VanithaKumari Scientist F, SSES, CSTD, MMG, IGCAR, Kalpakam, India	Biomimicry- Nature Inspired Surface Modification of Materials
12.00 - 12.50 PM	Prof. C. Rakkappan Head, Department of Physics, Annamalai University, Chidambaram, India	Core shell structures of nanoparticles for efficient enhancement of properties
12:50 -01:30 PM	<b>Lunch Break</b>	
01:30 – 02:20 PM	Mr. GeasinSavio Scientist (F) Defence Metallurgical Research Laboratory Defence Research & Development Organisation, India	"Ceramic Materials Used in Armour Applications"
02:20 - 03:30 PM	<b>Oral Sessions</b>	
03:30 - 04:00 PM	<b>Tea Break (End of Day 1)</b>	

**Programme Schedule – Day II**

Time (IST)	Speaker	Title of the Talk
<b>Day 2 (01.03.2023) –Online Mode</b>		
9:00 – 9:50	Prof. Ramamoorthy Ramesh Vice President for Research Professor of Materials Science and Nanoengineering, Rice University, USA	Materials Physics for Energy Applications
9:50 – 10:40	Prof. Dr. Aishah Abdul Jalil Centre of Hydrogen Energy, Institute of Future Energy Department of Chemical Engineering, Faculty of Chemical and Energy Engineering UniversitiTeknologi Malaysia, Malaysia.	Fibrous silica-based catalysts for methane dry reforming
10:40 – 11:00	<b>Tea Break</b>	
11:00 – 11:50	Dr Sindhuja Manoharan Faculty of Applied Energy Systems, Jeju National University , South Korea	"Electrochemical Energy Devices"
11:50 – 12:40	Dr. D. Paul Joseph Associate Professor Department of Physics National Institute of Technology, Warangal,INDIA	"Nano-dimensional thin films for optoelectronic and energy harvesting devices"
12:40 to 1:30	<b>Lunch Break</b>	
1:30 to 2:30	<b>Poster Session</b>	
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**Oral Presentation Details****Day 1: 28.02.2023 (Hybrid Mode)**

ORAL NUMBER	NAME	INSTITUTION	TITLE
ON001	AARTHI GANESAN	Justice Basheer Ahmed Sayeed College for Women (Autonomous), Chennai	Dipole Photoionization Of 5d Subshell Of Atomic Mercury Using Quantum Many-Body Relativistic Computational Approximation
ON002	NISHALINI A	Bhaktavatsalam memorial college for women , Chennai	Crystal Structure Determination And Analysis
ON003	R.MAHALAKSHMI	Bhaktavatsalam Memorial College For Women, ,Chennai	Crystal Growth And Characterization Of 3-Methylquinolinium Malate Single Crystal
ON004	PAVITHRA S	Bhaktavatsalam memorial college for women, korattur, ambattur	Green Synthesis Of Silver Nanoparticles Using Nyctanthes
ON005	RENUKA DEVI RAVI	Queen Mary's College,	Fabrication And Characterization Of Biomaterials Incorporated CMC Scaffold For Skin Tissue Engineering Applications
ON006	JYOTI	VIVEKANANDA GLOBAL UNIVERSITY, JAIPUR	Optical Studies In Tio <sub>2</sub> -Zns Doped( Pmma) Nanocomposite Thin Films
ON007	J. JOSFEL FLORA	Anna University, Crystal Growth Centre, Chennai	Ferrite Based Nanostructures For Uric Acid Sensing
ON008	YUVASHRI R	Queen Mary's College(A), Chennai	Synthesis, Structure Elucidation, Molecular Interaction Analysis, And Molecular Docking Studies Of A Curcumin Derivative:1-(4-Chlorobenzoyl)-3,5-Bis((E)-3,4-Dimethoxybenzylidene) Piperidin-4-One





ORAL NUMBER	NAME	INSTITUTION	TITLE
ON009	ANISH FATHIMA A	Queen Mary's College (A) chennai	SYNTHESIS, CHEMICAL AND PHYSICAL CHARACTERIZATION OF A CURCUMIN DERIVATIVE: 1-(4- Chlorobenzoyl)-3, 5- Bis ((E)-4-Methoxybenzylidene) Piperidin-4- One
ON010	HARI PRIYA. M	Quaid- E- Millath Government College For Women , chennai	Green Synthesis Of Metal Nanoparticles Using Aerva Lanata And Application
ON011	J M THOUFEEQ	Department of Medical Physics, College of Engineering, Anna University, Chennai	Digital Image processing of Confocal Fluorescence Polarization images for probing the microenvironment of metabolome NADH
ON012	J. GAYATHRI	Department of Medical Physics, College of Engineering, Anna University, Chennai	Dual nature of piperine as a drug and facilitator for drug binding efficacy.
ON013	N.DHARSINI	Government Arts College for Men, Nandanam, Chennai	Anticancer herbal drug: A short investigation
ON014	YASMIN	Department Of Applied Sciences And Humanities, Anna University, MIT Campus, Chennai	Synthesis And Enhanced Luminescence Properties Of Cr <sup>3+</sup> Doped Gahnite (ZnAl <sub>2</sub> O <sub>4</sub> ) For Red Emission Applications.
ON015	K. SIVARANJANI BABU	PG Department of Physics, Bhaktavatsalam Memorial College for Women.	Insilico evaluation of medicaments in the newly formulated topical patch against the wound healing repressor protein
ON016	JAYAMITHRA M P	Bhaktavatsalam Memorial College for Women, Chennai	Inhibitory Potential Of As-Synthesized Dressing Material Against Microbes



**Day 2: 01.03.2023 (Online Mode)**

ORAL NUMBER	NAME	INSTITUTION	TITLE
ON017	R G VAIDYA	UNIVERSITY COLLEGE OF SCIENCE, TUMKUR UNIVERSITY, TUMKUR	MODIFICATION IN THE ONSET OF UMKLAPP PROCESSES IN GAN
ON018	ATCHAYA	Ethiraj women's college ,	Synthesis And Characterization Of La <sub>2</sub> -xHo <sub>x</sub> Femno <sub>6</sub> Double Perovskite Compound
ON019	V.USHANANDHINI	Ethiraj college for women , Chennai	Ab_Initio Structural And Electronic Properties Of Aginse <sub>2</sub> Using Wein 2k Code
ON020	ADLINE BENILA S	Scott Christian College(Autonomous), Nagercoil,	The Crucial Role Of Fuel-To-Oxidant Ratio On Lanthanum Ferrites Synthesized By Sol-Gel Auto-Combustion Route
ON021	KALAISELVI D	Ethiraj college for women, Chennai	Studies On La <sub>2</sub> -Xybfemno <sub>6</sub> Double Perovskite
ON022	R SWETHA SHREE	Ethiraj College For Women, Chennai	Ab-Initio Structural And Electronic Properties Of Double Perovskite K <sub>2</sub> agincl <sub>6</sub> Using Wein2k Code.
ON023	VENKATARAHUL RG	RAJALAKSHMI ENGINEERING COLLEGE, THANDALAM.	MATERIAL HANDLING ROBOT WITH PATH PLANNING
ON024	S. KAVIYA	Ethiraj college for women (Autonomous) Chennai	PHASE STABILIZATION ON LA <sub>2</sub> -XDYXFEMNO <sub>6</sub> DOUBLE PEROVSKITE COMPOUNDS



ORAL NUMBER	NAME	INSTITUTION	TITLE
ON025	MARY SHAJINA S	Ethiraj college for women (Autonomous) Chennai	Green Synthesis Of Gold Nanoparticles, Mediated By The Fruit Extract Of Citrus Limon (Lemon), And Its Characterization
ON026	AARTHY V	Ethiraj college for women (Autonomous) Chennai	Ab-Initio Structural And Electronic Properties Of Agins2 Using Wein2k Code
ON027	C SIVADHARSHINI	Ethiraj college for women (Autonomous) Chennai	Stabilization Of Phase And Studies On La2-Xndxfemno6 Double Perovskite Compound
ON028	SUMITHRA R	Ethiraj college for women (Autonomous) Chennai	Ab-Initio Study Of Structural Properties Of Bese Using Optimised Lattice Parameter Using Wein2k Code.
ON029	VIJAYALAKSHMI G	Ethiraj college for women (Autonomous) Chennai.	Ab-Initio Study Of Structural Properties Of Bete Using Optimised Lattice Parameter Using Wein2k Code.
ON030	SRILAKSHMI RANGANAAYAKE E. S	Ethiraj college for Women	Ab-Initio Structural And Electronic Properties Of Double Perovskite K2aginbr6 Using Wein2k Code
ON031	SANTHOSH KUMAR BALU	<i>Dwaraka Doss Goverdhan Doss Vaishnav College, Chennai</i>	Magneto-dielectric response in TbMnO <sub>3</sub> at Room Temperature
ON032	SYED AZFARUL HAQUE	Netaji Subhas University, Jamshedpur	The characterization of unidirectional and woven palm fiber, cane fiber, sun grass reinforced with epoxy resin composites



**Poster Presentation Details**  
**Day 2 :01.03.2023 (Online Mode)**

POSTER NUMBER	NAME	INSTITUTION	TITLE
PN001	Dr.Z.Delci SARANYA V SUBHASHREE B R	PG Department of Physics, Dwaraka Doss Goverdhan Doss Vaishnav College, Chennai	A Photocatalytic performance of third order NLO active NiO- CdO nanocomposite green synthesized using Psidiumguajava leaf extract
PN002	ESWARI THULASIMUTHU	National Centre for Nanoscience and Nanotechnology, University of Madras, Guindy campus, Chennai - 25	Enhancing The Antioxidant, Antidiabetic and Antibacterial Properties of Curcumin Coated Zinc Oxide Nanoparticles
PN003	S.THARANI	SRM INSTITUTE OF SCIENCE AND TECHNOLOGY,KATTAN KULATHUR,POTHEI.	Hydrothermally treated Tungsten Oxide as an effective cathode for deep cyclable Aqueous Zn-Ion Battery Application.
PN004	HARINI LOGANATHAN	Ethiraj college for women, Chennai -8	Structural and Optical properties of Gd doped ZnO nanoparticles by chemical co- precipitation method
PN005	BLESSY REBECCA P N	SRM Institute of Science and Technology, Kattankulathur	Synthesis of ZnO/Graphene/Zif 8 Nanocomposites for the Non- Enzymatic Detection of Glucose
PN006	NAVEEN T B	SRM Institute of Science and Technology, Kattankulathur	Stabilizer-free MAX phase inks and Screen Printing of micro- supercapacitors
PN007	ATHULYA P.M.	Ethiraj college for women, Chennai -8	Structural and Optical properties of Gd doped ZnO nanoparticles by chemical co- precipitation method
PN008	SATHISH KUMAR PARAMASIVAM	University of Camerino, Italy	Dirac cones in bosonic spectra
PN009	RAKSHITHA D.E	Ethiraj collage for women (Autonoums)	Condensed matter physics and material
PN010	RAKSHANA . S	Ethiraj College For Women, No. 70, EthirajSalai, Chennai 600008	Evaluation of solubilization of Curcumin by bio-compatible poly(vinylpyrrolidone) and poly ethylene glycol matrix



POSTER NUMBER	NAME	INSTITUTION	TITLE
PN011	KIRUBA SAKTHI B	University of Madras, Guindy campus, Chennai 600025 600025	Crystallite Size Effect on Nano-CaWO <sub>4</sub> Indirect Conversion X-Ray Sensors
PN012	V. PAVITHRA	Ethiraj college for women, 70, EthirajSalai, Egmore, Chennai 600008, Tamilnadu, India	Novel polymer composite with carbon nanoparticles as Photocatalyst
PN013	ABINAYA S	Ethiraj college for women, Egmore, Chennai	Organic dye/ carbon nanomaterials chemically modified electrode for electrochemical sensing application
PN014	ROGINI G	Ethirajcollge for women , EthirajSalai, Chennai,	Green synthesis and characterization of ZnO nanocomposite with novel polymer.
PN015	AISHWARYA K	Ethiraj College for women, Chennai.	Evaluation of Mixed micellar system of Sodium dodecyl sulfate/ Sodium Cholate: a fluorescence probing approach
PN016	R AJOMIA	DR.M.G.R EDUCATION AND RESEARCH INSTITUTE UNIVERSITY	Ultrasonics Investigations On The Interactions Of Cleaning Agents With Human
PN017	K. THILAGA	Sri.S.Ramasamy Naidu Memorial College	Crystal Growth, Structural, Morphological, Optical, Mechanical, Magnetic and Electrical Investigations on Cesium Sulphate-Doped 4-Methoxyaniline: A Single Crystal for NLO and Antimicrobial Applications
PN018	L. SARUMATHI	Krishnasamy college of science, arts and management for women, Cuddalore	The ionic conductivity of bio-polymer poly vinyl alcohol with Indian medicinal plants – Acalypha indica and potato extract for electrochemical devices application
PN019	RICIA MARGARET. S	Ethiraj College for Women, Chennai- India	Synthesis and characterization of silver nitrate doped cyclodextrin nanosponges





POSTER NUMBER	NAME	INSTITUTION	TITLE
PN020	RESHMINA TONY A	Ethiraj College for Women, Chennai, India	A Study on the Influence of Calcination Temperature on the Structural and Optical Properties of Spinel Magnesium Ferrite Synthesized by Co-Precipitation Technique
PN021	SAKSHI JOSHI. A	Ethiraj College for Women, Chennai, India	Influence of GO and rGO on the Structural and Optical Properties of ZnO Photoelectrodes for Energy Harvesting Applications
PN022	SRAVANTHI R	Ethiraj College for Women, Chennai, India	A Computational Investigations of 1H Cyclopenta(B)Pyridine-DFT, Molecular, Electronic and Molecular Docking Analysis
PN023	POOJITHA.V	Ethiraj College for Women, Chennai, India	Synthesis and structural characterisation of ba doped bismuth ferrite
PN024	SILVIYA N	Ethiraj College for Women, Chennai, India	Nickel and its Oxide Nanocomponents: An Overview



## CORE – SHELL STRUCTURE OF NANOPARTICLES FOR UNIQUE PROPERTIES ENHANCEMENT

Dr. C. RAKKAPPAN\*

*Prefessor and Head, Dept. of Physics, Annamalai University, Chidhambaram – 608 002*

### Abstract

Multimodal nanoparticulate materials are described, offering magnetic, Photocatalysis and fluorescent imaging capabilities to exploit the complementary advantages of electrochemical and photodegradation. Ce-doped  $\text{Fe}_3\text{O}_4@ \text{NaYF}_4$  is successfully synthesized via the ethanothermal method. They comprise  $\text{Ce}:\text{Fe}_3\text{O}_4@ \text{NaYF}_4$  core/shell nanoparticles (NP's) with different cation dopants in the shell or core, including  $\text{Ce}:\text{Fe}_3\text{O}_4@ \text{NaYF}_4$ . These NP's are stabilized by Sodium hexameta Phosphate (SHMP) and Poly vinyl pyrrolidone (PVP). The properties of the prepared particles are studied by X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM), transmission electron microscopy (TEM), Fourier transform infrared (FTIR), UV–Vis Spectroscopy (UV-Vis), Photoluminescence spectroscopy (PL), X-ray photoelectron spectroscopy (XPS) and electrochemical methods. It has been found that the Ce element doped into the  $\text{Fe}_3\text{O}_4$  lattice resulting in lattice distortion, which can refine the grain and improve the crystal surface's integrity significantly. Transmission electron microscopy (TEM) confirmed the correlation of the crystallites shape and size with the experimental conditions, pointing to critical Ce content around 3% for the preparation of uniformly shaped grains, while fine coated  $\text{NaYF}_4$  content leads to monodispersity. In addition, shell coating of  $\text{NaYF}_4$  on  $\text{Fe}_3\text{O}_4$  can increase the particle size crystal, cause a red shift of the UV –Vis absorption, stretching vibration band, enhance binding energy of Fe–O and the chemical stability of the  $\text{Fe}_3\text{O}_4$  crystal. Studies of the magnetic behavior of nanoparticles shows the transition to superparamagnetic (SPION's) which helps to enhance the biomedical applicability. The photodegradation activity is also enhanced due to this Core/Shell formation of NP's.



## CRYSTAL STRUCTURE DETERMINATION AND ANALYSIS OF 3-(4- methoxyphenyl)-5- (4- benzyloxyphenyl)- 6-methyl-2- cyclohexen-1-one

A. Nishalini<sup>1\*</sup> & S. Sathya<sup>2</sup>

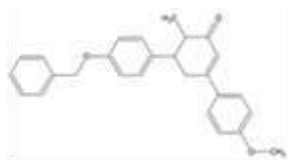
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<sup>2</sup> Department of Electronics & Communication Science/ Physics  
Shree Chandrabrabhu Jain College Minjur-601 203, India

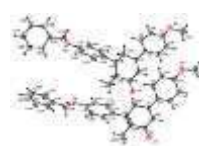
Email: [ssathyashanmugam991@gmail.com](mailto:ssathyashanmugam991@gmail.com)

### Abstract:

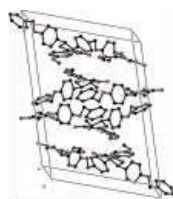
Chalcones are important constituents of many natural products. They are abundant in edible plants where they are considered to be the precursors of flavonoids and isoflavonoids. As part of our studies to examine the compounds in this series, we determined the crystal structure of the title compound. The title compound crystallized in Monoclinic space group  $P2_1/c$ . with unit cell parameters  $a = 20.5663 (12)\text{\AA}$ ,  $b = 15.2878 (9)\text{\AA}$ ,  $\beta = 07.938 (4)^\circ$   $c = 14.5689 (8)\text{\AA}$ , and  $V = 4358.0 (4)\text{\AA}^3$ . The structure was solved by direct methods using the program SHELXS-97 and refined by SHELXL-97 with full-matrix least-squares procedure. The cyclohexene ring adopts an envelope conformation. In addition to the van der Waals interactions, the molecular structure of the compound is stabilized by C-H...O type hydrogen bonds. The crystal packing is stabilized by the van der Waals interactions in addition to C-H... $\Pi$  inter molecular hydrogen bonds.



Chemical diagram



ORTEP PLOT



Packing diagram



## Modification in the onset of Umklapp processes in GaN

Bommalingaiah B.<sup>1,2</sup>, Narayan Gaonkar<sup>2</sup>, R. G. Vaidya<sup>2\*</sup>

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### Abstract:

GaN is one of the binary III-V nitrides with direct bandgap semiconductor characterized by built-in spontaneous and piezoelectric polarization fields[1]. The investigations of lattice thermal conductivity including the macroscopic polarization effects are very rarely reported[2–8]. This work is motivated in the view of investigations the effect of polarization fields on the scattering processes and understanding the behavior of lattice thermal conductivity. In the present work, the lattice thermal conductivity of GaN is theoretically investigated including the split transverse phonon dispersion in the presence of macroscopic polarization fields. The macroscopic polarization effects show significant increase in the magnitude of lattice thermal conductivity. The modified phonon group velocity and Debye temperature due to spontaneous polarization is found to affect the onset of Umklapp processes. Our numerical calculations of thermal conductivity including macroscopic polarization fields explain the observed experimental data.

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3. A. Jeżowski, O. Churiukova, J. Mucha, T. Suski, I. A. Obukhov, and B. A. Danilchenko, *Mater. Res. Express* **2**, 085902 (2015).
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## GREEN SYNTHESIS OF SILVER NANOPARTICLES USING NYCTANTHES ARBOR – TRISTIS LEAF EXTRACT

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### Abstract:

In recent years, the green synthesis of nanoparticles (NPs) using plant extracts is now recognised as an effective method for producing metallic NPs, particularly silver, copper, and gold NPs, since it entails a quick, simple, low-cost, and environmentally friendly bioprocess. In the current study, silver nanoparticles were synthesised by reducing a 1 mM silver nitrate solution with leaf extract from *Nyctanthes arbor-tristis*. The method is proved to be incredibly simple, inexpensive, and efficient. The synthesis of the nanoparticles was confirmed visibly, in which the colourless solution turns into a brown-colour solution. The synthesized silver nanoparticles from *Nyctanthes arbor-tristis* leaf extract were analysed by using UV-visible spectroscopy and FT-IR. Silver nanoparticles synthesized from *Nyctanthes arbor-tristis* leaf extracts showed highest peaks at 425 nm.





## **Fabrication and Characterization of Biomaterials incorporated CMC scaffold for skin tissue Engineering Applications**

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<sup>1</sup>National Centre for Nanoscience and Nanotechnology, University of madras, Guindy campus, Chennai-25, India.

<sup>2</sup>Queen Mary's College, Chennai - 600004, India.

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### **Abstract:**

The attention of science and technology in nanoparticles are getting accelerated for its various applications across the world. The goal of this study is to fabricate the biomaterials incorporated CMC scaffold for skin tissue engineering. Skin, the largest sense organ plays vital role in protecting from external atmosphere. To increase the mechanical strength and biological properties of the scaffold, biomaterials such as collagen, gelatin and PVA were added. Here, glutaraldehyde were used as a cross linker in the prepared nanocomposite. To determine the thermal stability and functional groups present in the nanocomposites were determined by TGA and FTIR analysis. The biological properties were determined through cytotoxicity, hemolysis and antibacterial activity. The structural morphology of the nanocomposite reveals the stable, regular and fibrous structure which was examined by SEM analysis. Fibroblast cells were used to study the biocompatibility of the scaffold and cross-linked scaffold. An MTT result shows that both the scaffolds are biocompatible with higher cell viability. The obtained results confirmed that the prepared scaffold is hydrophilic and had significant tensile properties. The obtained results revealed that the developed scaffolds in this work have the potential to use as skin substitute.



## Synthesis and characterization of $\text{La}_{2-x}\text{HO}_x\text{FeMnO}_6$ double perovskite compounds

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### ABSTRACT

The double perovskite system involves the strong interplay between crystallographic orientation of constituent elements and electronic and magnetic properties. The advantage of exchanging lanthanides and transition metal ions make the double perovskite structured material yield with the important prospectus for the study towards application. The double perovskite material  $\text{La}_{2-x}\text{HO}_x\text{FeMnO}_6$  ( $x=0, 0.2, 0.4$ ) has been phase stabilized using conventional solid-state reaction. Energy dispersive spectra confirm the presence of La, HO, Mn & O elements in prepared compound. The structural stability of prepared compounds is confirmed using XRD studies which confirm the oxidation state of HO, La, Fe & Mn. the formation of double perovskite structure is confirmed using the powdered X ray diffraction by  $\text{HoFeO}_3$ . This compound reveals the antiferromagnetic properties from  $\text{Fe}^{3+}$  and  $\text{Mn}^{3+}$  magnitude of magnetic moment aligned anti parallel to each other. To analyze morphology and elemental properties of prepared  $\text{La}_{2-x}\text{HO}_x\text{FeMnO}_6$  ( $x=0,0.2,0.4$ ) compounds the scanning electron microscopy technique with energy dispersive spectra (EDS) distribution of fine grain from the SEM micrographs of pure and La substituted  $\text{HO}_{2-x}\text{FeMnO}_6$  compounds. The EDS analysis confirms the presence of HO, La, Fe, Mn and O elements in prepared  $\text{La}_{2-x}\text{HO}_x\text{FeMnO}_6$  ( $x=0, 0.2, 0.4$ )

**KEYWORDS:** Double perovskite Compounds, Solid state reaction, X-ray diffraction, FE-SEM



## Optical studies in TiO<sub>2</sub>-ZnS doped( pmma) nanocomposite thin films

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### Abstract:

Nanotechnology focuses on creating and utilizing materials with nanoscale dimensions; nanoparticles have a high surface area to volume ratio and, as a result, very unique properties. The TiO<sub>2</sub>-ZnS nanoparticles (NPs) doped Poly (methyl methacrylate) (PMMA) nanocomposite thin films were prepared at room temperature using the solution cast method. With their wide energy gap, inorganic TiO<sub>2</sub> NPs enable the creation of modified polymer composites with novel optical properties that can be altered by adjusting the inorganic material's composition, concentration, and size. Considering their potential use in optoelectronic devices, TiO<sub>2</sub> NPs are very intriguing materials. During the preparation of the nanocomposite films, the dopant concentration of TiO<sub>2</sub>-ZnS NPs was fixed at 0.5, 1, 1.5, and 2%. The structural and morphological properties of these nanocomposite films were characterised by X-ray diffraction (XRD), Scanning Electron Microscope (SEM), and Fourier Transform Infrared (FTIR) Spectroscopy. The optical parameters such as, dispersion, band-gap energy was determined by UV-visible Spectroscopy by analyzing the samples in transmittance and reflectance mode.

**Keywords:** TiO<sub>2</sub>-ZnS nanoparticles, PMMA, nanocomposites, solution casting method, optoelectronic devices.

### References

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## Ferrite based nanostructures for uric acid sensing

Josfel Flora John<sup>1</sup>, Durgalakshmi Dhinasekaran<sup>2</sup>, Shanthi Subashchandran<sup>1\*</sup>

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<sup>2</sup>*Ethiraj College for Women, Egmore, Chennai-600 008, India*

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### Abstract:

High levels of uric acid in the human body leads to increased risk of type 2 diabetes, cardiovascular disease and Lesch-Nyhan syndrome. The end product of metabolic breakdown of purine in human body is uric acid. Hence, early detection will be helpful to prevent the development of the disease. Earlier methods of uric acid analysis use the chemical oxidation of uric acid to allantoin producing tungsten blue chromophoric compound. Later, enzymatic sensors using the enzyme uricase (UOx) were used for the analysis which suffers from selectivity and stability of the electrode material. Other methods include liquid chromatography, titration and spectrophotometry which have the disadvantages of requirement of expensive equipment, overestimation of uric acid concentration and in situ electrode performance is not possible. To overcome these drawbacks, non-enzymatic biosensors based transition metals made of ternary compounds called ferrites are better alternatives as they are robust, cost-effective, abundant and easy to synthesise. Here-in we report ferrite-based biosensor for uric acid detection via electrochemical method. The structural, morphological and functional analysis of the ferrite nanostructures was analysed. The chemical kinetics of the electrode/electrolyte were studied through electrochemical impedance spectroscopy. Cyclic voltammetry at various concentrations of the analyte was performed to understand the mechanism of the UA oxidation. The amperometric response obtained was used to calculate the sensitivity, limit of detection and limit of quantification of the fabricated biosensor. The ferrite biosensor showed high sensitivity towards UA and selectivity in the presence of interferents. In conclusion, the reported ferrite based non-enzymatic UA sensor is a potential candidate which can be used in clinics to detect UA in patients with improved accuracy.



# Synthesis, Structure Elucidation, Molecular Interaction Analysis, And Molecular Docking Studies of a Curcumin Derivative:1-(4-Chlorobenzoyl)-3,5 Bis((E)-3,4-Dimethoxybenzylidene) Piperidin-4-One

R. Yuvashri<sup>1</sup>, A. Anish Fathima<sup>1</sup> and G.Usha<sup>1\*</sup>

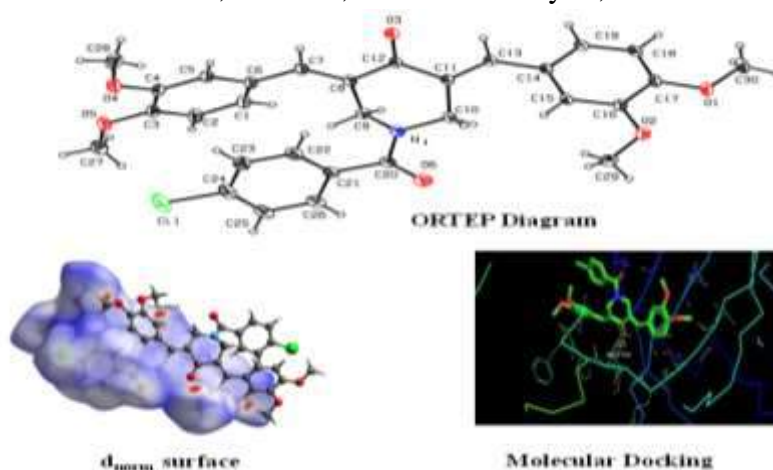
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## Abstract:

Curcumin is one of the important components of the curcuminoids family, originally derived from Curcumin Longa. It is the most effective nutraceuticals to exist, with a unique molecular structure giving it powerful properties as an anti-oxidant, anti-inflammatory, anticancer, antimicrobial, etc. A novel Curcumin derivative 1-(4-chlorobenzoyl)-3,5-bis((E)-3,4-dimethoxybenzylidene) piperidin-4-one (CDMBP) has been synthesized by Claisen-Schmidt condensation reaction method. CDMBP single crystal was successfully grown from acetone by slow evaporation method at ambient temperature. The crystal structure of the compound was derived by Single Crystal X-ray Diffraction studies (SCXRD). The title compound CDMBP was crystallized in a triclinic crystal system with a P T space group. Hirshfeld surfaces were generated to visualize and quantify short contacts, regions of varying potentials, and C-H... $\pi$  interactions. 2D fingerprint plots were also analyzed, in which the contribution due to H...H contact to the total Hirshfeld surface was found to be the most significant with 42.2%. Molecular docking stimulation for 1M17 protein was performed and it revealed that the ligand fits well at the active site of the target protein with binding energy - 11.35.

**Keywords:** Curcumin derivative, SCXRD, Hirshfeld Analysis, Molecular docking Analysis



## SYNTHESIS, CHEMICAL AND PHYSICAL CHARACTERIZATION OF A CURCUMIN DERIVATIVE: 1- (4-Chlorobenzoyl)-3, 5- Bis ((E)-4-Methoxybenzylidene) Piperidin-4-one

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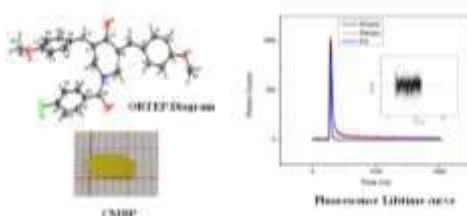
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### Abstract:

A novel Curcumin derivative 1-(4- Chlorobenzoyl)-3, 5- Bis ((E)-4-Methoxybenzylidene) Piperidin-4-one (CMBP) has been synthesized by Claisen-Schmidt condensation method. CMBP single crystal was successfully grown from acetone by slow evaporation method at ambient temperature. The crystal structure of the compound was derived by Single Crystal X-ray Diffraction studies (SCXRD). The title compound CMBP was crystallized in a monoclinic crystal system with centrosymmetric P 2<sub>1</sub>/c space group. From NMR analysis, the various types of proton and carbon atom present in the title compound has been studied. From UV-Vis spectral analysis the cutoff wavelength, and linear optical constants such as the absorption coefficient, band gap, extinction coefficient, refractive index and reflectance were calculated. The Photoluminescence spectrum of the grown crystal has been studied and it shows peaks at 501 nm, and 708nm which belongs to the green and red emission radiation region respectively. Fluorescence spectrum profile endorsed the electronic transitions and photophysical properties of CMBP. The modes of vibrations of different chemical groups present in the title compound CMBP were identified using Fourier Transform Infrared spectral analysis (FTIR). The third-order nonlinear optical property (NLO) of CMBP was investigated in detail using a Z-scan technique with He-Ne laser at 632.8 nm as laser source. The nonlinear optical susceptibility ( $\chi$ ), absorption coefficient ( $\beta$ ) and refractive index (n) were calculated using transmittance data.

**Keywords:** NMR, UV-Vis spectral analysis, FTIR, Photoluminescence, Fluorescence, Z-Scan,

### Graphical Abstract:



## Ab-initio Structural and Electronic properties of double perovskite $K_2AgInBr_6$ using wein2k code

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### Abstract:

The double perovskites generate lead-free, non-toxic, and stable materials for renewable energy applications such as solar photovoltaics and light-emitting diodes (LEDs) as thermoelectric (TE) generators. The cubic phase double perovskite crystal structure  $K_2AgInBr_6$  has a lattice parameter of 10.32Å and belongs to the space group of  $Fm\bar{3}m(225)$ . Density functional theory has been used to examine the structural and electrical thermoelectric properties of double perovskite  $K_2AgInBr_6$ . The  $K_2AgInBr_6$  has an ideal band gap for solar cells with a large absorption energy band in the visible region. The band gap of 1.37 eV is computed from the band structure of  $K_2AgInBr_6$ .





## GREEN SYNTHESIS OF METAL NANOPARTICLES USING AERVA LANATA AND APPLICATION

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### Abstract:

High potential of metal nanoparticles spot light considerable attention in various applications in the material, optical, electronics, and energy industries. Rather than traditional chemical methods of synthesizing metal nanoparticles, biosynthesis of metal nanoparticles using microorganisms, plant parts extract, pay way for many research innovations. Green synthesis of diverse metal nanoparticles has recently been demonstrated using plant parts extract, which provides several advantages over the traditional chemical synthesis methods. The aim of green synthesis is mild temperature -less energy, non-toxic chemicals and reagents are needed, diverged metal nanoparticles are synthesized, environmental friendly, more sustainable and cost-effective techniques. The metal nitrates [Strontium nitrate, barium nitrate and cobalt nitrate] were reacted with flower extract of Aerva Lanata to form metal oxide nanoparticles, where Avera Lanata acts as a reducing agent. Further, the synthesized nanoparticles were characterized; the crystalline structure of the green synthesized metal nanoparticles was studied from their XRD patterns. The FTIR spectral analysis provides the information regarding the formation of crystal-line nanoparticles and the presence of functional groups in the sample. UV-visible absorption spectroscopy acts as a primary characterization tool for the study proved the formation of nanoparticles. The morphology of the nanoparticles were found using Scanning Electron Microscopy (SEM). These nanoparticles prepared through green synthesis method, are promising candidate in various applications like biomedical and catalytical degradation.



## Digital Image processing of Confocal Fluorescence Polarization images for probing the microenvironment of metabolome NADH

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### Abstract

Reduced form of Nicotinamide adenine dinucleotide (NADH) is an enzyme cofactor that takes part in oxidation-reduction reactions of cellular metabolism. Alterations in NADH concentrations is associated with changes in metabolic reactions and disease prognosis. Fluorescence anisotropy is widely used to monitor the microenvironment of biomolecule of interest. Several parameters like micro-viscosity, size of biomolecule can be predicted from rotational diffusion rate of fluorophore during the lifetime of excited state. The micro-viscosity of biomolecule could be used as a biomarker for disease diagnosis. In this work we use fluorescence polarization images of MCF7 breast cancer cell lines and chicken muscle Tissues sliced to few microns thickness to calculate the distribution of anisotropy values in the samples. 405nm diode laser is used for excitation and emission is obtained from 410nm to 500nm which predominantly belongs to NADH emission region. The mean anisotropy values of MCF7 cell lines and tissue sections were found to be 0.15794 and 0.1891. The higher mean anisotropy value of NADH in tissue sections indicates that rotation of fluorophore is more restricted than in adherent cell lines due to highly organized embedding matrix in tissues and higher micro-viscosity.



## Dual nature of piperine as a drug and facilitator for drug binding efficacy

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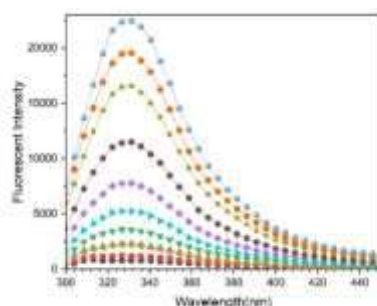
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### Abstract

Many researchers have done their analysis in the drug binding interaction with proteins, which has a significant role in the pharmacokinetics. There are variety of drugs are currently available in drug delivery system. Still there is a need in improvement of interaction mechanism that to prove the total binding of drug, to reduce the unbound sites, to load accurate protein sites. This issue can be improved by the addition of a nano material or another drug. There are many dual drugs such as cytarabine, 5-azacytidine, doxorubicin and etc are available to treat various diseases. The common Indian spices like turmeric and pepper have the organic molecules respectively. We have studied the binding of Curcumin and Piperine using quantum mechanical simulation and spectroscopic analysis. In this study we have carried out the spectroscopic analysis to provide an evidence for the effect of piperine to improve the binding efficacy of curcumin with milk protein. The result of the UV Vis spectroscopy reveals that binding efficacy with milk protein was increased when piperine concentration is minimized compared with curcumin. Fluorescence spectroscopy reveals that steady quenching done as piperine with decreased concentration in curcumin binded protein complex. Therefore increased drug solubility can cause occurrence of improved drug binding interaction to the protein. Here piperine is used as a drug and also as a facilitator to improve Curcumin- Protein drug binding interaction.

**Key words:** Curcumin, Drug binding Interaction, Piperine, Fluorescence quenching.



## Anticancer herbal drugs: A short investigation

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### Abstract

Cancer is a frightful disease and represents one of the biggest health care issue for the human race and demands a proactive strategy for cure. Mortality increases day by day on occurrence of cancer in human. There are many type of cancer such as sarcoma, lymphoma, leukaemia, and carcinoma which are currently treated by chemotherapy, brachytherapy, radiotherapy, hormone therapy, etc. In this context pharmaceutical research plays an important role with the quality of herbal medicine. Worldwide scientists turn up their focus into herbal medicine to boost up the immune system and to cure deadly disease without side effects. The antioxidant rich flora species helps to protect our cells from reactive oxygen species (free radicals). There is a source of novel chemical entities of therapeutic utility due to the vast structural diversity observed in them. The efficacy of these plant drugs can also be enhanced the inoculation of Nano particles in it. 'HERBS AS DRUGS' cause potential pharmacokinetic interaction mechanism on human body. Hence some of the anticancer herbal drugs and its advantages are summarised in this review.

**Keywords:** Anticancer, Herbal drugs, Nano particles, Summary.



## Synthesis and enhanced luminescence properties of Cr<sup>3+</sup> doped Gahnite (ZnAl<sub>2</sub>O<sub>4</sub>) for red emission applications

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### Abstract:

Zinc aluminate nanophosphors have a number of potential applications, particularly in the fields of lighting and displays. They have been studied for use in LED lighting, as their high efficiency and long lifetime make them a promising alternative to traditional phosphors. In addition to their optical properties, zinc aluminate nanophosphors have also been investigated for their catalytic properties. This paper describes the sol gel combustion synthesis of Cr<sup>3+</sup> doped ZnAl<sub>2</sub>O<sub>4</sub> (ZAC) particles. A thorough investigation was conducted to comprehend the interaction of dopant (Cr<sup>3+</sup>) and ZnAl<sub>2</sub>O<sub>4</sub> host matrix, as well as the influence of doping on their structural, optical, and luminescence characteristic properties. The powder samples were thoroughly characterized using XRD, UV–Visible Diffuse Reflectance, and Photoluminescence spectroscopic techniques. The XRD analysis demonstrates the cubic structure formation with space group Fd-3m of polycrystalline nanoparticles, as well as a decrease in crystallite size with increasing Cr<sup>3+</sup> concentration. The mean crystallite size varied from 18 to 22 nm. SEM and EDS showed uniform composition and microstructure of the ZnAl<sub>2-x</sub>Cr<sub>x</sub>O<sub>4</sub> powders. The band gap energy red-shifted as Cr<sup>3+</sup> was incorporated into the host matrix. The diffuse reflectance spectra show two absorption peaks at 381 nm and 527 nm are assigned to the <sup>4</sup>A<sub>2g</sub> → <sup>4</sup>T<sub>1g</sub> and <sup>4</sup>A<sub>2g</sub> → <sup>4</sup>T<sub>2g</sub> characteristic transitions of Cr<sup>3+</sup> ions. The PL emission spectrum, on the other hand, shows four distinct peaks, indicating the manifestation of Cr<sup>3+</sup> ions in octahedral symmetry, that is, Cr<sup>3+</sup> ions in a strong crystal field. Doping Cr<sup>3+</sup> in host matrix resulted in luminescence enhancement when compared to the host material. Overall, zinc aluminate nanophosphors are a promising material with a wide range of potential applications in various fields. Ongoing research continues to explore their properties and potential uses.



## **Insilico evaluation of medicaments in the newly formulated topical patch against the wound healing repressor protein**

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### **Abstract:**

Inhibition of proteins that delay the wound healing process would fasten the healing process. A downstream negative regulation of the Wnt signaling pathway by the enzyme, Glycogen synthase kinase – 3 $\beta$  would cause the phosphorylation and subsequent degradation of  $\beta$ -catenin.  $\beta$ -catenin, is one of the active proteins that involve wound healing gene expression and other cofactors at the nuclear level. The present work studied the Glycogen synthase kinase – 3 $\beta$  inhibition efficiency of embedded active ingredients in the formulated biodegraded, bio-waste-based epidermal patch. Six active molecules had been screened off for the drug-likeness based on Lipinski's rule and toxic filters. The six screened-off ligands were 3-Methoxy Hexane, Butyric acid, 2-Methyl 4-Heptanol, Imidazole and 10, 12-Tricosadiyonic acid. Among the six filtered compounds, Nopyl acetate showed the highest binding affinity with the minimal energy of -6.1 Kcal/mol, an inhibition constant of 0.04 mM. Molecular dynamics and simulation studies with 100 ns on the complex of Nopyl acetate confirm the binding stability. Insilico analysis implied that the formulated wound dressing material would be efficient to accelerate the wound healing process through the inactivation of Glycogen synthase kinase – 3 $\beta$ .



## Ab-initio Structural and Electronic Properties of AgInSe<sub>2</sub> using wein2k code

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### Abstract:

The structural and electronic properties have been calculated for AgInSe<sub>2</sub> using Density Functional Theory (DFT). AgInSe<sub>2</sub> is one of the potential compounds of this family of alloys due to its wide band gap of around 1.2eV. This chalcopyrite structure is closely related to the zinc blend structure. It forms the crystal structure with the space group I 42d. Its lattice parameters are  $a=6.56\text{\AA}$ ,  $b=6.56\text{\AA}$ , and  $c=12.65\text{\AA}$ . It shows the direct energy gap with  $E_g \sim 1.2\text{eV}$ . The electrical studies of this compound give a wide range of conductivity and it is also dominated by shallow donors. The band gap lies between 0.8 and 2.0eV. The total and partial density of states indicates the state of the compound has a strong contribution of valance band in the energy range from 1.873eV to 1.92eV.





## The crucial role of fuel-to-oxidant ratio on lanthanum ferrites synthesized by sol-gel auto-combustion route

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### Abstract:

Substantial effort has been devoted to fabricate lanthanum ferrites via the sol-gel auto-combustion route at a sintering temperature of 900° C for three hours. The fuel-to-oxidant (F/O) ratio was the crucial parameter for regulating the structure and morphology of synthesized perovskite. Proliferating the fuel-to-oxidant ratio has given the ability to control the growth and agglomeration of nanoparticles.

The prepared lanthanum ferrites were systematically investigated by X-ray diffraction (XRD), Diffuse reflectance spectroscopy (DRS) and a High-resolution scanning electron microscope (HRSEM). XRD revealed that all the prepared samples have shown an orthorhombic phase with phase group *Pnma*. Furthermore, the average crystallite decreases from 56 nm to 46 nm with the increasing F/O ratio. Consequently, an opposite trend has been seen in the surface area and it went from 18.91 – 19.9 m<sup>2</sup>/g.

DRS suggested a marginal increase in the band gap and the average band gap was found to be 2.1 eV. HRSEM profoundly showcased increased agglomeration of nanoparticles. These findings exhibited that the prepared samples find their application as active visible-light-driven photocatalysts in wastewater treatment.



## Studies on $\text{La}_{2-x}\text{Yb}_x\text{FeMnO}_6$ double perovskite materials

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### Abstract:

The cubically ordered double perovskite compound,  $\text{La}_{2-x}\text{Yb}_x\text{FeMnO}_6$  ( $x=0,0.2,0.4$ ), has been synthesized using high temperature solid state reaction method. Powder x-ray diffraction data indicates the formation of  $\text{La}_{2-x}\text{Yb}_x\text{FeMnO}_6$  ( $x=0,0.2,0.4$ ). It also has wide application potential in magnetic, electrical optical and thermal application. XRD, UV-vis DRS and VSM were used as analytical techniques. XRD pattern recorded for the prepared sample confirms the formation of the double perovskite materials. Hence, double perovskite  $\text{La}_{2-x}\text{Yb}_x\text{FeMnO}_6$  ( $x=0,0.2,0.4$ ). Compounds prepared at high temperature are characterized for their structural optical and magnetic properties. UV-DRS talks about the reflectance spectrum of the material. VSM reveals the antiferromagnetic property of the material.

**Keywords:** Double perovskite Compounds, X-ray diffraction, UV-DRS, VSM



## Ab-initio Structural and Electronic properties of double perovskite $K_2AgInCl_6$ using wein2k code

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### Abstract:

The double perovskites are the potential materials for renewable and clean energy. The cubic phase double perovskite crystal structure  $K_2AgInCl_6$  has a lattice parameter of 10.32Å along with the space group of  $Fm\bar{3}m(225)$ . The structural and electronic properties of double perovskite  $K_2AgInCl_6$  have been investigated using density functional theory. The crystal structure of  $K_2AgInCl_6$  is highly stable and has a direct band gap, which is important for inter-band transitions and recombination. The band gap of 2.34 eV was computed from the band structure of  $K_2AgInCl_6$ .



## Material Handling Robots With Path Planning

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### Abstract

Automatic Material Handling Robot (AMHR) was designed and fabricated which can be used in industrial applications to move materials around a manufacturing facility or warehouse. The reason is to overcome the logistic problems that often occurs in the workplaces and to make improvement to the facilities provided in the workplaces. In the industries or factories, the AMHR can ease the physical strain on human workers by performing tiring tasks, such as lifting and carrying heavy materials, more efficiently with no signs of fatigue creeping in. This Vehicle can be used to transport many different types of material including pallets, rolls, racks, carts, and containers. It excels in applications as repetitive movement of materials over a distance, regular delivery of stable loads, Medium throughput volume, when on-time delivery is critical and late deliveries are causing inefficiency, operations with at least two shifts, etc.

**Key words:** Robots, Industrial Application, Physical Strain, Materials.



## PHASE STABILIZATION ON $\text{La}_{2-x}\text{Dy}_x\text{FeMnO}_6$ DOUBLE PEROVSKITE COMPOUNDS

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### Abstract:

A Phase Pure double perovskite material provide flexible selection of ions and the combination of La, Fe, Dy and Mn provide an interesting prospect. The double perovskite  $\text{La}_{2-x}\text{Dy}_x\text{FeMnO}_6$  was synthesized using conventional high temperature solid-state reaction technique. Crystal structure, optical and magnetic properties of these double perovskite materials were described. XRD, UV-DRS and VSM were used as analytical technique. The x-ray powder diffraction (XRD) patterns at room temperature indicates the formation of  $\text{La}_{2-x}\text{Dy}_x\text{FeMnO}_6$  compounds, having single phase cubic structure. Analysis of UV-DRS is based on the absorption of ultraviolet light or visible light by chemical compounds, which results in the production of distinct spectra. Also VSM is an instrument used to measure the magnetic moment, the most fundamental quantity in magnetism, of solid samples.

### Keywords:

Solid State Reaction, X-ray diffraction, UV-DRS, VSM.



## Green Synthesis of Gold Nanoparticles, mediated by the Fruit Extract of Citrus limon (Lemon), and its Characterization

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### Abstract:

Synthesis of nanoparticles through green route has acquired a great momentum in recent times. Replacing the toxic chemicals by plant extracts for the reduction of metallic nanoparticles has received more attention as they provide a safer, cost-effective and ecofriendly approach to produce nanoparticles with greater stability and varied dimensions. This paper presents a novel method for successful reduction of gold nanoparticles through Citrus limon (lemon) fruit extract. The lemon extract served both as reducing and stabilizing agent under ambient temperature. The formed gold nanoparticles were characterized using X-ray diffraction which confirms the crystalline face centered cubic phase with Fm3m space group. SEM micrographs show the existence of gold nanoparticles embedded in a lime extract matrix. UV-visible reflectance spectrum further substantiated the phase formation by showing three bands, two in the visible and one in near infra-red region. The characteristic stretching modes of carboxylic acid and amine groups present in the FTIR spectrum validate the bio reduction and stabilization of gold nanoparticles. Good zones of inhibition obtained on assays of bacterial and fungal strains establish the prepared gold nanoparticles to be an effective antimicrobial agent.



## Ab-initio Structural and Electronic Properties of AgInS<sub>2</sub> using wein2k code.

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### Abstract:

The structural and electronic properties of AgInS<sub>2</sub> have been calculated using Density Functional Theory (DFT). The Full Potential Linear Augmented Plane Wave (FP-LAPW) method is used to obtain the Self Consistent Field (SCF). The lattice parameter of the tetragonal crystal structure, AgInS<sub>2</sub> is  $a=b=5.52 \text{ \AA}$  and  $c=11.08 \text{ \AA}$  along with the space group I-42d. The chalcopyrite semiconductor AgInS<sub>2</sub> core/shell structures generate intense narrow-band photoluminescence originating from a band-edge transition. The total density of states and partial density of states indicate that the state of the compound has a strong contribution to the valence band in the energy range from -10 up to 0.0 eV. The electronic band gap of ternary semiconductor AgInS<sub>2</sub> is found to be 1.9 eV. The electronic band structure shows that AgInS<sub>2</sub> is a direct band gap semiconductor at  $\Gamma - \Gamma$  point.





## Stabilization of phase and studies on $\text{La}_{2-x}\text{Nd}_x\text{FeMnO}_6$ double perovskite compound

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### Abstract:

The double perovskite compound  $\text{La}_{2-x}\text{Nd}_x\text{FeMnO}_6$  [X=0, 0.2, 0.4] which follows cubic system of arrangement has been synthesized using high temperature solid-state reaction technique. These kind of double perovskite compounds like  $\text{La}_{2-x}\text{Nd}_x\text{FeMnO}_6$  [X=0, 0.2, 0.4] are gaining importance due to their flexible ability in the selection of ions and vast application potential in magnetic, optical, electrical and thermal application. The structure of crystal, optical and magnetic properties of these double perovskite materials were described. XRD, UV-DRS and VSM were used as analytical techniques. The powder X-ray diffraction data shows the formation of  $\text{La}_{2-x}\text{Nd}_x\text{FeMnO}_6$  [X=0, 0.2, 0.4] compound, having single phase cubic structure. UV-DRS gives information about the reflectance spectrum of the material. VSM reveals the ferromagnetic property of the material.

### Keywords:

Solid State Reaction, X-ray diffraction, UV-Vis DRS, VSM.



## Inhibitory potential of as-synthesized dressing material against microbes

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### Abstract:

Any damage occurs in the tissue of the body either internally or externally causes wounds. The occurrence of the wounds incurs the invasion of micro-organisms. The association of the micro-organisms with the wounds has the real impact on healing wounds and not their mere existence around the wound site. Acute or chronic wounds are susceptible to a medley of aerobic and anaerobic micro-organisms. Molecular docking, a tool to find the computer simulation of the conformation of a receptor-ligand complex has been employed in the research domain of proteins structure and functions and drug designing. In the present work, a wound dressing material was synthesized from physiologically chicken fibrin, fish scale collagen, ethanol extract of *Mangifera indica* (L.) and spider web. The compounds present in the wound dressing material were identified by GCMS analysis. Two gram positive, two gram negative, one fungus were used for docking together with nitrofurazone as the standard and the docking results concluded that the two gram positive showed the best inhibition on the wound dressing material.



## Ab-initio Study of Structural properties of BeSe using optimised lattice parameter using wein2k code

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### **Abstract:**

The structural properties for BeSe have been calculated using the full potential linearized augmented plane wave (FP-LAPW) method using wein2k code. The BeSe compound has ideal cubic structure with space group F-43m (216). The position co-ordinate for Be (0,0,0) and Se (1/4,1/4,1/4) with the optimized lattice parameters are  $a=b=c=4.647 \text{ \AA}$  and  $\alpha=\beta=\gamma=90^\circ$ . To obtain the optimized lattice parameter, volume versus energy graph is plotted. Using the optimized lattice constant, bulk modulus ( $B_0$ ) and pressure derived of the bulk modulus ( $B'$ ) can be obtained. BeSe is an indirect bandgap semiconductor.



## Ab-initio Study of Structural properties of BeTe using optimised lattice parameter using wein2k code

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### Abstract:

The structural properties for BeTe have been calculated using the full potential linearized augmented plane wave (FP-LAPW) method using wein2k code. The BeTe compound has ideal cubic structure with space group F-43m (216). The position co-ordinate for Be (0,0,0) and Te (1/4,1/4,1/4) with the optimized lattice parameters are  $a=b=c=5.146 \text{ \AA}$  and  $\alpha=\beta=\gamma=90^\circ$ . To obtain the optimized lattice parameter, volume versus energy graph is plotted. Using the optimized lattice constant, bulk modulus ( $B_0$ ) and pressure derived of the bulk modulus ( $B'$ ) can be obtained. BeTe is an indirect bandgap semiconductor.



## SYNTHESIS AND CHARACTERIZATION OF SILVER NITRATE DOPED CYCLODEXTRIN NANOSPONGES

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### Abstract

Water bodies are polluted on daily basis through different sources by various kinds of pollutants. Dye is one of the major pollutants that is used by industries for wide range of purposes. Textile industries use different kinds of dyes and indigo carmine is one of them that is used. Cyclodextrin nanosponges are materials that are apt to absorb pollutants due to its cyclic structure and the pores created during the synthesis due to the cross linkers added. Doping of silver nitrate makes it more efficient in absorption of pollutants. Fourier transform infra-red spectroscopy (FTIR), scanning electron microscope (SEM), energy dispersive spectroscopy (EDAX), Thermo gravimetric analysis (TGA), UV visible spectroscopy are the various characterizations that were done for the silver nitrate cyclodextrin nanosponges. The silver nitrate doped cyclodextrin nanosponges shows better absorption efficiency compared to undoped cyclodextrin nanosponges.

**Keywords:** Nanosponges, Cyclodextrin, Water Pollution



## Influence of GO and rGO on the Structural and Optical Properties of ZnO Photoelectrodes for Energy Harvesting Applications

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### Abstract

Graphene and its derivatives are materials that appear in almost every research area nowadays, and is shining star due to its intrinsic outstanding physiochemical properties. Owing to high electron movability, a lot of interest is shown in utilizing the zinc oxide (ZnO) as photoelectrode in such applications. In this study, graphene oxide (GO) and reduced graphene oxide (rGO) are synthesised through a simple modification of Hummer's method. As-synthesised GO and rGO are doped with ZnO, which are used as precursors to deposit thin films on glass substrates using the spin coating method. The structural, optical, and electrical properties of both the synthesised samples and thin films are investigated in detail. The X-ray diffraction (XRD) is used for structural characterization, which confirmed the hexagonal wurtzite crystal structure. The increasing GO and rGO weight percentage has resulted in increasing the crystallite size, and in turn, decreased the resistivity. All the films exhibit transmittance around 90% in UV-Visible region, which make them useful as an optical window in optoelectronic applications. High-resolution scanning electron microscope images are used to examine the variation in microstructures following the insertion of GO and rGO.

**Keywords:** ZnO, GO, rGO, thin films, photoelectrodes

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## A Photocatalytic performance of third order NLO active NiO-CdO nanocomposite green synthesized using *Psidium guajava* leaf extract

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### Abstract:

In water purification, to remove its organic pollutants by the method of using catalysts is called Photocatalysis. Recently, metal oxide semiconductors with larger surface area are widely used as catalysts for the degradation of toxic dyes because they possess an excellent combination of photochemical activity, thermal and mechanical stability. NiO-CdO nanocomposite was fabricated biologically using *Psidium guajava* leaf extract without adding additional chemical precipitating agents. The phytochemicals present in the *Psidium guajava* leaf extract acts as potential reducing agent to produce stable NiO-CdO nanocomposite. The FT-IR spectrum and XRD studies confirm the presence of functional groups and the structure of NiO-CdO nanocomposite. The SEM images of the NiO-CdO nanocomposite clearly confirmed the existence of nanoneedles. Z-scan studies confirmed that the title composite exhibited appreciable third order NLO properties. The calculated nonlinear refractive index values of the NiO-CdO nanocomposite was found to be  $5.24 \times 10^{-9} \text{ cm}^2/\text{W}$ . The high value of NLO susceptibility possessed makes the NiO-CuO nanocomposite highly polarized. The occurrence of the reverse saturable absorption (RSA) effect from the Z-scan studies confirmed that the composite is well suited for nonlinear optical and photonic devices. Photocatalytic tests confirmed that the green synthesized NCs effectively degraded RhB dye under visible light. After 90 min light irradiation, the NiO-CdO nanocomposite catalysts removed 86 % dye molecules. The obtained results confirmed that the NiO-CuO nanocomposite seems to be an effective non-toxic photocatalyst for degrading toxic dyes with better third order NLO properties.

**Keywords:** Nanocomposite, Green synthesis Leaf extract, SEM, Z-scan

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## Enhancing The Antioxidant, Antidiabetic and Antibacterial Properties of Curcumin Coated Zinc Oxide Nanoparticles

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### Abstract:

This article explains the antioxidant, antidiabetic and antibacterial properties of the Curcumin coated Zinc Oxide nanoparticles which were synthesized by the wet chemical method. The body's defence mechanisms often require support in preventing the effects of oxidative stress and Diabetes mellitus (DM) is a complex metabolic disease characterized by a high glucose level due to either insufficient insulin or insulin resistance. Curcumin-coated zinc oxide has the ability to overcome all those complications. The photoluminescence property of curcumin is used to analyse the impurities and the photocatalytic performance of the prepared sample. The prepared sample was characterised by UV, XRD, Photoluminescence, RAMAN, FTIR and SEM. By examining the Alpha-amylase and alpha-glucosidase assay, it shows approximately 92% and 89% of Inhibition. The photoluminescence of the prepared sample was excited at 450 nm, which corresponds to the highest peak and Curcumin-coated Zinc Oxide nanoparticles act as an excellent property for oxidative stress. Antimicrobial assays were conducted against both Gram-negative and Gram-positive bacterial stains. The synthesized curcumin-coated zinc oxide nanoparticles exhibit good antioxidant properties. The results of this investigation demonstrate that the as-synthesized nanoparticles can act as an effective and also hold promises for many other biomedical applications.



## Hydrothermally treated Tungsten Oxide as an effective cathode for deep cyclable Aqueous Zn-Ion Battery Application

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### Abstract:

Tungsten oxide ( $\text{WO}_3$ ) based transition metal oxide is a potential cathode for Aqueous Zinc Ion Battery (AZIB) application. But due to its poor stability and low capacity, it's further battery application is affected. In order to improve the stability of  $\text{WO}_3$ , herein we have investigated Water-in-salt electrolytes (WISEs) and designed a Zn-  $\text{WO}_3$  battery. WISEs usage is limited due to their high cost but in this work, we will discuss some cheap and simple WISEs, which can be easily produced.  $\text{WO}_3$  has been synthesized by hydrothermal method and analyzed through techniques such as XRD (X-ray Powder Diffraction), SEM (Scanning Electron Microscope) and UV DRS (UV- vis Diffuse Reflectance Spectroscopy). The electrochemical studies were carried out for the WISEs to check their specific capacity, energy density, power density and capacity retention for about 100 cycles. Furthermore, we have constructed a Zn- $\text{WO}_3$  battery with different WISEs without adding any additives, demonstrating great potential for the next-generation energy storage application.

**Keywords:** Aqueous Zinc Ion Battery (AZIB), Water-in-salt electrolytes (WISEs), Transition Metal oxide, Sustainable electrolyte.

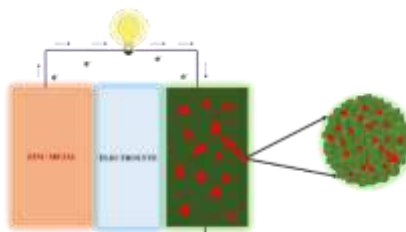


Fig: SCHEMATIC ILLUSTRATION OF Zn- $\text{WO}_3$  battery

## Structural and Optical properties of Gd doped ZnO nanoparticles by chemical co-precipitation method

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### Abstract:

The facile co-precipitation method was employed to prepare Pure and Gadolinium (Gd) doped Zinc Oxide (ZnO) nanoparticles (NPs) with the precursors Zinc acetate dihydrate and Gadolinium trinitrate in higher dopant ratios (3mol%, 4mol%, and 5mol %). The structural properties of synthesized pure and Gd doped ZnO NPs were investigated by X-Ray Diffractometer which showed a high degree of crystallinity of the sample. The diffraction peaks (100), (002), and (101) are indexed to the hexagonal wurtzite structure and the lattice parameters and crystallite size of the prepared NPs were analyzed. Morphological properties were studied by HR-SEM, and the optical studies of the material were analyzed by UV-Visible spectroscopy technique for the exploration of the absorption and transmission of the nanoparticle material.

**Keywords:** ZnO; Co-precipitation; nanoparticles

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## Synthesis of ZnO/Graphene/Zif 8 Nanocomposites for the Non-Enzymatic Detection of Glucose

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### Abstract:

The growing number of diabetes mellitus cases around the world has received great attention from the research and pharmaceutical and clinical industries. Diabetes mellitus can be controlled and monitored based on the level of glucose in the blood. Commercially available glucose sensors are based on the catalytic activity of the enzymes immobilized on a substrate. However, the enzymatic sensors have the disadvantage of instability and thus non-enzymatic detection of glucose was needed. Fourth-generation sensors based on metal oxides and nanostructure metals have been promising electrode materials for the direct electro-oxidation of glucose due to the electrocatalytic activity towards glucose. Among them, ZnO is widely exploited as a non-enzymatic glucose sensor due to its non-toxicity, electrocatalytic activity and biocompatibility. Incorporating the MOF into metal oxides increases the catalytic activity and functional sites but they have limitations due to their low conductivity. Nanocomposites of metal oxides with metals, and carbon-based materials like graphene, and carbon nanotubes have been reported in the recent literature for increasing the conductivity of the electrochemical sensor. Owing to its large surface areas, porous structure, electrocatalytic activity and conductivity, the prepared material can be used in the electrochemical sensing of glucose in real samples.



## Stabilizer-free MAX phase inks and Screen Printing of micro-supercapacitors

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### Abstract:

This research work demonstrates the screen printing technology to fabricate the micro-supercapacitors using two-dimensional vanadium carbide ( $(V_2Al_2)C_3$ ) based MAX phase inks without using any stabilizer or binary-solvent systems (Shown in Fig.1). The conductive tracks of the micro-supercapacitors were developed on the plastic as well as paper-based substrates with high printing resolution and spatial uniformity, which are determined by the series of characterization tools including SEM, viscometer and source meter analyses. The capacitance and energy density of the  $(V_2Al_2)C_3$  based MAX phase printed micro-supercapacitors showed a higher rate than existing active materials. The screen printing technique provides a promising way for developing flexible storage devices for large-scale fabrication and easy-to-integrate components of printable electronics.

**Keywords:** MAX phase; Micro-supercapacitors; Screen Printing Technology; Vanadium Carbides; Energy Storage Devices

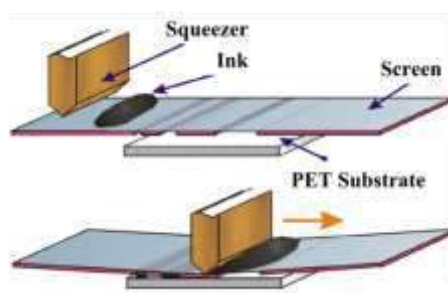


Figure 1. Screen Printing of MAX phase ink on Substrate

## Dirac Hamiltonians for bosonic spectra

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### Abstract

Dirac materials are of great interest as condensed matter realizations of the Dirac and Weyl equations. In particular, they serve as a starting point for the study of topological phases. This physics has been extensively studied in electronic systems such as graphene, Weyl, and Dirac semimetals. In contrast, recent studies have highlighted several examples of Dirac-like cones in collective excitation spectra, viz. in phonon, magnon, and triplon bands. These cannot be directly related to the Dirac or Weyl equations as they are bosonic in nature with pseudounitary band bases. We address this issue by constructing a generic deformation scheme that maps any fermionic Hamiltonian and its spectrum to that of a bosonic problem. In particular, we show that any Dirac-like equation can be deformed into a suitable bosonic form. The resulting bosonic spectra bear a two-to-one relation to that of the parent Dirac system. Their dispersions inherit several interesting properties including conical band touching points and a gap-opening role for ‘mass’ terms. The relationship also extends to the band eigenvectors with the bosonic states carrying the same Berry connections as the parent fermionic states. The bosonic bands thus inherit topological character as well. If the parent fermionic system has nontrivial topology that leads to midgap surface states, the bosonic analog also hosts surface states that lie within the corresponding band gap. The proposed bosonic Dirac structure appears in several known models. In materials, it is realized in  $\text{Ba}_2\text{CuSi}_2\text{O}_6\text{Cl}_2$  and possibly in  $\text{CoTiO}_3$  as well as in paramagnetic honeycomb ruthenates. Our results allow for a rigorous understanding of Dirac phononic and magnonic systems and enable concrete predictions, e.g., of surface states in magnonic topological insulators and Weyl semimetals.



## Evaluation of solubilization of Curcumin by bio-compatible polyvinylpyrrolidone and poly ethylene glycol matrix

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### Abstract

Curcumin (CUR) is a well-known Indian cooking ingredient which is now used as an established pharmaceutical agent. The medicinal qualities of CUR range in many fields varying from being a simple anti-inflammatory agent to anticancer and anti-HIV agent. It has also been used in other neurological diseases such as Alzheimer's and Parkinson's diseases. For the treatment of cancer, CUR is tried as a photosensitizer (PS) in photodynamic therapy. For the effective administration of a PS molecule, transdermal route of drug administration has profound advantage. To have a good penetration of the drug molecule, it is possible to use bio-compatible polymers. CUR is generally fluorescent in nature and owing to its hydrophobicity; dissolution studies with various drug delivery systems are done using fluorescence spectroscopic techniques. In the present work, the solubilization of CUR is achieved by using poly vinyl pyrrolidone (PVP) and poly ethylene glycol (PEG) as the drug delivery systems. The binary polymer system of PVP and PEG has been evaluated as a possible solubilizer for CUR. The pre-formulation studies of ternary system of CUR-PVP-PEG are carried out in the further process and evaluated as a successful drug delivery system.

**Keywords:** Curcumin, poly vinyl pyrrolidone, polyethylene glycol, penetration enhancer, solubilization, drug delivery system.

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## Crystallite Size Effect on Nano-CaWO<sub>4</sub> Indirect Conversion X-Ray Sensors

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### Abstract

X-ray imaging is a powerful analytical tool that is commonly used as a medical diagnostic technique in the health care industry. As X-rays are ionizing, there is a constant need to monitor their effects [1]. Therefore, X-ray sensors are used to measure the dose and the local radiation exposure. Hence, this work focuses on developing highly sensitive indirect conversion X-ray sensors. Here, the X-rays are converted to visible photons by means of a scintillator and the visible light is converted to photocurrent using a photodiode [2]. Calcium tungstate (CaWO<sub>4</sub>) is a promising scintillating material and it was selected to develop indirect conversion sensors for low-dose X-rays (mGy). It was synthesized by the chemical precipitation method and the product was subsequently calcinated at four different temperatures to get four crystallite sizes (18, 19, 25, and 63 nm). Samples were characterized for phase and morphology then applied to fabricate sensors. The observed linear dose-dependent sensitivity explores the possibility of utilizing nano-CaWO<sub>4</sub> for device development. These experimental findings will be discussed with a suitable mechanism in detail.

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## NOVEL POLYMER COMPOSITE WITH CARBON NANOPARTICLES AS PHOTOCATALYST

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### Abstract

Nanoparticles have excellent solubility, reactivity, adsorptive and photocatalytic properties. Particles can also be used in cancer treatments and other biomedical applications. Carbon nanoparticles having a diameter size less than 100nm exhibit excellent photoluminescent efficiency which lead to their application in photocatalytic activity. Now a days, the green chemistry approach should be favoured and carbon nanoparticles has been reported in many article studies using different precursors from natural and waste sources by hydrothermal, microwaves, ultrasonic, solvothermal, pyrolysis, electrochemical and so on. The current study on synthesis of carbon nanoparticles using banana peel extract which led to their application in photocatalytic activity. The extract led to rapid ,simple and eco- friendly study the biosynthesis of carbon nanoparticles. A simple method for Preparing a polymer flim containing polymer doped carbon nanoparticles. The carbon nanoparticles and polymer flim were characterized using UV, Photo luminescence, XRD, SEM methods.

**Keywords:** carbon nanoparticle, doped polymer, Nanocomposite, banana peel, photocatalyst.



## Organic Dye/Carbon nanomaterial Chemically modified electrode for electrochemical sensing application

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### Abstract

Hydrogen sulphide ( $H_2S$ ) is a colourless gas which is toxic, corrosive, and flammable. Hydrogen sulphide detection and sensing is an area of interest from both an environmental and a biological perspective. While many methods are currently available, the most sensitive and applicable ones are electrochemical based.  $H_2S$  is produced naturally in crude petroleum, natural gas, food by bacterial breakdown of human and animal waste. Here, we report Methyl Violet immobilised carbon nanotube modified electrode (GCE/CNT) for electrochemical sensing of  $H_2S$  in pH 7 phosphate buffer solution (PBS). Different carbon nanomaterials like Graphene oxide, Carbon nanotube, Activated carbon, Graphite nanoparticle modified glassy carbon electrodes were subjected to the 500  $\mu M$  of  $H_2S$ . In which methyl violet immobilized carbon nanotube showed excellent sensing efficiency. Further studies are done using MV@CNT/GCE modified glassy carbon electrode. The effect of scan rate MV adsorbed on CNT/GCE modified system showed adsorption controlled reaction. The effect of the  $H_2S$  concentration on the CV of MV@CNT/GCE yielded a linear increase in the oxidation peak current ( $i_{pc}$ ) in the range from 100  $\mu M$  to 6.5 mM with the sensitivity of 1.25mA/ $\mu M$ .



## Green synthesis and characterization of ZnO nanocomposite with novel polymer

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### Abstract:

ZnO is a well-known semiconductor material that can be synthesized in the form of nanoparticles or quantum dots which have wide applications in photocatalytic dye degradation, fluorescence studies, and many other applications because of their relative non-toxicity. The Green synthesis of ZnO nanocomposite was done using *Eclipta alba* which was confirmed by the UV-Visible absorption study which indicated the absorption at a wavelength of 340nm. The Photocatalytic dye degradation of ZnO nanocomposite was studied using methylene blue. Similarly, polymer-incorporated ZnO nanocomposite solution was also subjected to the photocatalytic activity of dye degradation. The thin film formed with the polymer-incorporated ZnO nanocomposite was also studied. ZnO nanocomposite and polymer-incorporated ZnO nanocomposite were screened for UV-Visible absorptions. Morphology and size were monitored using SEM and XRD data. From the UV absorption, the photocatalytic dye degradation of ZnO nanocomposite was studied. From this study, we can confirm that the ZnO nanocomposite acts as a photocatalyst.

**Keywords:** ZnO nanocomposite, *Eclipta alba*, Polymer incorporated, Photocatalyst.



## Evaluation of Mixed micellar system of Sodium dodecyl sulfate/ Sodium Cholate: a fluorescence probing approach

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### Abstract

Surface active agents are wonder molecules which can be used in variety of applications, like in cosmetic industry, pharmaceutical industry, food industry. They can be used as self-associated organized media by aggregation of single micelle or they can also prepared as mixed micelles. Mixed micelles find applications as drug-delivery nanocarriers, chemotherapeutic agents. The characterization and study of mixed micelles of Sodium dodecyl sulfate (SDS) and Sodium cholate (NaC) by fluorescence probing have been carried out. The present work studies the polarity inner core and the nature of micelle-water interface of mixed micelles of SDS/NaC by fluorescence probing. Here, 8-Anilino-naphthalene-1-sulfonic acid (ANS) were used as fluorescent probe. ANS is a hydrophobic drug molecule, having importance in a pharmaceutical agent. ANS is considered as fluorescent probe with an emission peak at 520 nm. The solubilization of hydrophobic ANS by surfactant and bile salt was achieved and the nature of association of ANS with surfactant and bile salt, namely SDS and NaC was evaluated.

**Keywords:** Mixed micelles, sodium dodecyl sulfate, bile salt, ANS, fluorescence probing.

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# Crystal Growth, Structural, Morphological, Optical, Mechanical, Magnetic and Electrical Investigations on Cesium Sulphate-Doped 4-Methoxyaniline: A Single Crystal for NLO and Antimicrobial Applications

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## Abstract

A new single crystal of cesium sulphate-doped 4-methoxyaniline (CS-4MOA) was obtained by the solvent evaporation approach. XRD manifests that the CS-4MOA crystallizes in orthorhombic crystal structure. SEM-EDAX analysis was performed to examine the surface morphology and the composition of CS-4MOA sample. Ultraviolet-visible spectral study validates the transparency of CS-4MOA in the region of 330-1100 nm. The mechanical stability of CS-4MOA crystal was assessed through Vickers microhardness analysis. VSM analysis was used to evaluate the magnetic behaviour of the CS-4MOA crystal. The electrical characteristics of the CS-4MOA were investigated by impedance study for various temperatures. The NLO parameters of CS-4MOA were computed by the Z-scan technique. The existence of second-order nonlinear optical susceptibility in CS-4MOA was confirmed by the SHG investigation. Additionally, the antimicrobial activity of CS-4MOA was performed against bacterial strains and fungal pathogens for medicinal applications.

**Keywords:** CS-4MOA; single crystal; SEM; SHG; Antimicrobial activity; microhardness; optical study



## A Computational Investigations of 1H Cyclopenta(B)Pyridine- DFT, Molecular, Electronic and Molecular Docking Analysis

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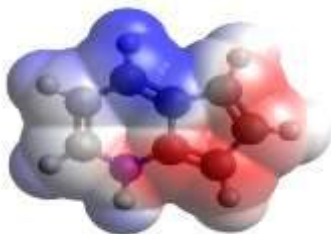
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### Abstract:

1H Cyclopenta(B)Pyridine is a pyridine derivative and it is theoretically examined using the DFT [1] method via B3LYP methods. The molecular structure and morphology of the title compound have been meticulously computed. Electrostatic potential map (ESP) and Fukui analysis are used to identify the presence of reactive zones, such as electrophilic and nucleophilic zones present in them. The various energy properties are computed using the energy differences between HOMO and LUMO [2]. The presence of non-covalent interaction (NCI) in the molecule is identified using the RDGmap. The pharmacological analysis shows the bioavailability of the compound and can be used as a drug because of its non-precarious behaviour. Molecular docking was used to investigate the biological activity of the title compound, which indicated that the title compound could have antiviral activity against SARS-COVID.

Keywords: DFT; NCI; Pyridine; ESP



**Keywords:** DFT; NCI; Pyridine; ESP

### References:

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## NICKEL AND ITS OXIDE NANOCOMPONENTS: AN OVERVIEW

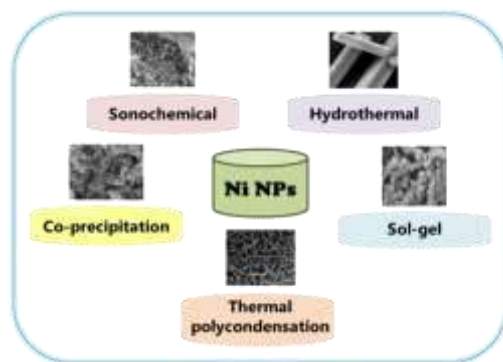
Silviya N<sup>1\*</sup> and Mahalakshmi S<sup>1</sup>

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### Abstract

The upcoming generations are responsible for creating less hazardous and environmentally beneficial substances. Metal oxide nanoparticles significantly fall under this non-toxic category and expresses predominant characteristics such as stability, high sensitivity, and selectivity. This article provides a review of the effects of synthetic techniques on particle size and shape, the changes in characteristics seen as particles go from bulk to nanoscale, and the role of doping in enhancing attributes in oxides of iron, manganese, nickel, zinc, zirconium, cobalt and copper. This work's primary focus is on how the characteristics of nickel oxide nanoparticles and their nanocomposites change when their synthesis process, size and dopants are altered. Nickel is more distinctive than other metals due to its great availability, low price and prominence in their optical, magnetic, electric and catalytic properties. A remarkable transformation in the shape and crystallite size of nanoparticles is evidenced by changing their calcination temperatures. Furthermore, when the calcination temperature rises, the Bandgap energy of NiO particles decreases and magnetic examination reveals that the magnetization value of NiO inevitably decreases as the calcination temperature rises. A discussion of how these nanocomponents can resolve current challenges and offer potential solutions concludes the overview.



**Keywords:** Nickel oxide, scanning electron microscope (SEM), dopants

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## A Study on the Influence of Calcination Temperature on the Structural and Optical Properties of Spinel Magnesium Ferrite Synthesized by Co-Precipitation Technique

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### Abstract

Spinel ferrites have sparked considerable interest among researchers due to their potential applications in a wide range of fields. Spinel magnesium ferrite was synthesized by the co-precipitation method and calcined at different temperatures. The influence of the calcination temperature on the structural and optical properties of the prepared magnesium ferrite was investigated through X-ray diffraction (XRD) and UV-Visible (UV-Vis) spectroscopy studies. The increase in crystallinity with increasing calcination temperature is demonstrated by XRD analysis, confirming the effect of calcination temperature on structural properties. Fourier-transform infrared (FTIR) spectra revealed tetrahedral and octahedral metal-oxygen stretching vibrations in spinel ferrites. UV-Vis studies were used to examine the optical properties of the prepared samples, and the variation in band gap energy with calcination temperature was also investigated. Scanning electron microscopy (SEM) images present an agglomerated morphology and Energy dispersive X-ray analysis (EDX) revealed the purity of the synthesized magnesium ferrite, showing the presence of only Mg, Fe and O elements.

**Keywords:** Spinel ferrites; Calcination temperature; Structural properties; Band gap;

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## SYNTHESIS AND STRUCTURAL CHARACTERISATION OF Ba DOPED BISMUTH FERRITE

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### Abstract

Ba doped bismuth ferrite nanoparticles having the general formula  $\text{Bi}_{1-x}\text{Ba}_x\text{FeO}_3$  were successfully synthesized by sol-gel method, using nitrates as starting material. Tartaric acid and polyvinyl alcohol were used as a chelating agent. The synthesized nanoparticle powder was sintered at three different temperatures at 550 C, 600 C, 650 C for 5 hours. Leaching with dilute nitric acid and distilled water is done to remove the impurities. The structural, optical, dielectric properties were determined using XRD, FTIR, VSM at room temperature. In Fourier transform infrared, the spectrum consists of various strong and weak bands around  $2450\text{-}500\text{ cm}^{-1}$ . In XRD, the crystalline size, lattice strain, dislocation density can be determined. In VSM, the P-E hysteresis loop confirms the ferromagnetic behavior of prepared nanoparticles. The Ba doped bismuth ferrite nanoparticles samples at room temperature, it indicates that the samples have potential candidates information storage devices for spintronic devices. For practical application, the magnetic properties may increase.

**Keywords:** Sol-gel method, hysteresis loop, ferromagnetic behavior, spintronic devices.

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## Dipole Photoionization of 5d Subshell of Atomic Mercury using Quantum many-Body Relativistic Computational Approximation

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### Abstract:

Photoionization is a basic process in the field of atomic spectroscopy which helps us to understand the dynamics of the system in atomic level. Probing the atomic system with an electromagnetic radiation reveals the characteristics of the atoms and many important phenomena. More than four decades photoionization studies on atoms and ions have been scrutinized by both experimentalist [1-2] and theoreticians [3-4]. The hydrogen atom is a single electron system which can be solved exactly for its wave function and energy levels. For many electron systems i.e. for the systems other than hydrogen atom the wave function of the subshells and the energy values cannot be solved exactly either analytically or numerically. This is because for higher Z atoms the interaction between the electrons from different configurations brings out the coulomb correlations and coulomb interactions between them. Calculating the coulomb correlations between the correlated electrons are highly impossible using analytical method. In this regard having two electrons is too many. The solution to solve many electron systems is to go for best approximation methods as the exact solutions do not exist. The approximation methods give us the transition matrix element which contains information about the atoms/ions under study. In the present work, the transition matrix element of 5d subshell of atomic mercury is calculated and the dipole photoionization parameters (i) 5d cross sections and (ii) angular distribution of 5d photoelectrons are derived using the many-body relativistic quantum computational approximation RRPA (Relativistic Random Phase Approximation) [5] and compared with the experimental data [6]. As mercury is a high Z atom, strong electron correlations are present between the electrons in different configuration. The influence of relativistic, correlation and truncation of inter-channel coupling effects on the photoionization parameters of inner 5d subshell of mercury are reported.

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## CRYSTAL GROWTH AND CHARACTERIZATION OF 3-METHYLQUINOLINIUM MALATE SINGLE CRYSTAL

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### **Abstract:**

A single crystal of 3-methylquinolinium malate (3MMA) was synthesized by slow evaporation and was subjected to nonlinear optical examination. The crystal was analyzed by single XRD and UV-visible spectroscopy. Single X-ray diffraction confirmed the geometry of monoclinic space group P21, a vital requirement for the NLO phenomena. UV-visible spectral examination found the wavelength of UV-cut off at 433 nm.



## Synthesis, optical, vibrational spectroscopy, experimental and Theoretical investigation of nonlinear optical properties of L-argininium Hydrogen squarate

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### Abstract

The compound of L-Argininium Hydrogen Squarate (LAHSQ) was grown by slow solvent evaporation technique at room temperature method. Structural investigation by single crystal XRD reveals that LAHSQ crystallizes in triclinic system with space group P1. Vibrational spectroscopic studies were performed by utilizing FT-IR spectral analysis along with DFT/B3LYP/6-311++G (d, p) method using GAUSSIAN 09 software. The molecular structure of LAHSQ crystal has also been optimised by using Density Functional Theory (DFT) using method with B3LYP/6-311++G (d, p) basis methods in order to find the whole characteristics of the molecular complex. The HOMO and LUMO energy results show that good exchange of charge happened inside the molecule. The electronic absorption spectrum of organic molecules that shows alteration due to the solvation processes was evaluated by TD-DFT in the gas and solvent phase in addition to the recorded UV-visible spectrum. Second harmonic generation (SHG) efficiency measurement was done to examine the enhancement in the nonlinear optical characteristics of the grown crystal.

**Keywords:** Single crystal, FT-IR, UV-Vis, NLO, DFT



## Spectroscopic Investigations of Thiamine Mononitrate Using Quantum Computational (DFT) And Experimental Methods

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### Abstract

The Fourier Transform Infrared and Raman spectra of thiamine mononitrate were recorded in the range 400-4000  $\text{cm}^{-1}$  and 2500-50  $\text{cm}^{-1}$  respectively in solid phase. A detailed vibrational spectral analysis has been carried out and assignments of observed fundamental bands have been proposed on basis of peak positions and relative intensities. The harmonic vibrational frequencies, bond length, bond angle and Mullikan atomic charge were also calculated by DFT method using 6-311G(d, p) basis set. The scaled theoretical frequencies showed very good agreement with experimental values. Thermo-dynamical parameters are calculated and interpreted. The experimental UV- Vis absorption spectrum was recorded in the range of 200-800 nm in chloroform. The theoretical electronic transitions for the title molecule in three solvents are computed using TD-SCF/B3LYP method with 6-311G (d, p) basis set. The NMR chemical shifts of  $^1\text{H}$  and  $^{13}\text{C}$  were computed and chemical shifts are analyzed. Using TD-SCF methods Frontier molecular orbitals, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the title compound are computed with same B3LYP/6-311G (d, p) method. The bonding and anti-bonding structure of the molecule were studied using NBO analysis.



## Hydrogen bonding study with FTIR in 1-hexanol with substituted benzaldehyde and substituted acetophenone

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### Abstract

FTIR spectroscopic method is used to study the H-bonding between substituted benzaldehyde and substituted acetophenone with hexanol in ccl4 .this work is concerned with Nash method the formation constant (K) of the 1:1 complexes is discussed. Alcohol group is proton donating ability and aldehyde group are proton accepting ability indicate the interaction of the complexes.



## Single crystal inspection, Hirshfeld surface investigation and DFT study of Propanone 2,4-dinitrophenyl hydrazone (PDNPH)

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### Abstract

“Propanone-2,4-dinitrophenyl hydrazone” (PDNPH) has been grown successfully with good optical quality in acetone solvent. The unit cell dimension and space group of grown PDNPH crystal were examined by single crystal X-ray diffraction technique. We present experimental and theoretical studies on the molecular structure, nonlinear optical (NLO), electronic structural and UV spectral analysis for the grown crystal was determined using the density functional method (DFT/B3LYP) with a basis set of 6–311G (d, p). The computed HOMO and LUMO energies, demonstrate that the charge transfer happens within the PDNPH molecule. The computed findings were used to generate the UV spectra and nonlinear optical behavior of PDNPH crystal which are in well accordance with the experimental results. Various inter contacts present within the crystal were visualized through 3-D molecular hirshfeld surface analysis and their percentage contribution towards the total hirshfeld surface area has been quantized using 2D finger print plot method.

**Keywords:** Single crystal; NLO; Hirshfeld surface analysis; DFT;



## **Introspective View on Growth, Electrical, Vibrational, Linear and Non Linear Optical Properties Of Benzimidazolium Salicylate Single Crystal**

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### **ABSTRACT**

A Dynamic nonlinear solitary crystal of benzimidazolium salicylate was harvested by employing Standard Slow Evaporation Technique. The structural framework of the titled material was obtained by employing Single Crystal X-Ray Diffraction technique. The Phase purity and Crystalline fineness were examined by the means of Powder Crystal X-Ray Diffraction analysis. The presence of functional groups and molecular footprint of the material were examined by the means of FTIR (Fourier Transform Infrared Spectroscopy) and FT- Raman. NMR study of benzimidazole compound constitutes a significant tool in understanding the molecular dynamics and the structural parameters. The dielectric responses and electrical conductivity measurements have been carried out for titled compound. The linear optical properties of the material were investigated by means of UV-VIS analysis. The Non-linear optical properties of the material were investigated by means of Kurtz Perry Powder Technique.

Keywords: NMR, FTIR, Kurtz Perry, XRD, Single crystal.





## Surface Morphology and Optical Properties of ZnS Nanocomposite Via Hydrothermal Method

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### Abstract

Zinc sulphide nanostructures have attracted increasing attention due to their potential applications in both conditional optical devices and new generation of nano-electronics and nano-optoelectronics because of their special structure – related chemical and physical properties. The investigation has been focused on the preparation and characterization of II–VI semiconductor nanoparticles for applications in biological field, photo- and electroluminescence properties because of their size-dependent (which is tunable) and have promising optoelectronic applications. Zinc sulphide is successfully synthesized by hydrothermal method at a temperature of about 220 °C. The product was obtained in powder form. The structure, composition and optical property of the resultant product were characterized by X-ray diffraction, Fourier transform infrared spectroscopy, Ultraviolet Visible spectroscopy, scanning electron microscopy, Photoluminescence and Energy dispersive X- ray analysis. At room temperature, the X-ray diffraction pattern shows that the prepared ZnS nanoparticles have a zinc-blended crystal structure. Fourier transform infrared spectroscopy showed that the chemical composition of the material possesses Zn-S stretching vibration. The nanoparticles in the scanning electron microscopy image have an average particle size of around 50 nm. The Photoluminescence emission spectra of ZnS nanocrystals excited at 300 nm consist of a broad band (340 nm–560 nm) characterized by two main contributions peaks at 420 and 530nm. The blue change in the band gap caused by the quantum confinement effect is visible in the ultraviolet absorption spectrum. The band gap of those samples has been calculated from absorption spectra and is found to be about 3.6 eV. Zinc is chosen for Hydrogen Evolution Reaction [HER] based on the volcano plot.

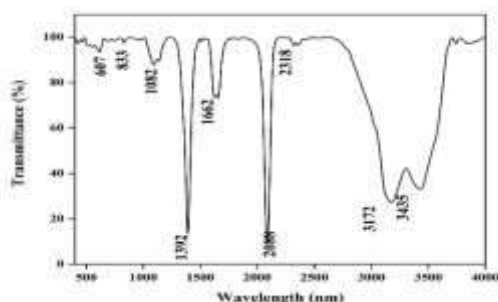


Fig: FTIR spectrum of ZnS

**Keywords:** Zinc sulphide, HER, Nanoparticles, Photoluminescence



## Spectroscopic studies of 5-(4-dimethylamino) benzylidene) pyrimidine - 2, 4, 6 (1H,3H,5H)-trione

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### Abstract

The chemical formula of 5-(4-diethylamino) benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione DBT crystal has been found to be C<sub>15</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>. The crystal consists of a benzene ring with three double bond oxygen and two NH bonds. The FTIR and FT-Raman, spectra of DBT has been recorded. In the FT-IR and FT-Raman spectra the NH band has been observed at 3452 cm<sup>-1</sup> and 3488 cm<sup>-1</sup> respectively. In FT-Raman spectrum the vibrational stretching of C-H bond has been noticed at 3081 and 3057 cm<sup>-1</sup>. FTIR band at 1638 cm<sup>-1</sup> indicates the presence of C=O stretching vibrations and in FT-Raman spectrum the C=O spectral vibrations has been registered at the region of 1754 and 1680 cm<sup>-1</sup>.

The <sup>1</sup>H and <sup>13</sup>C NMR spectra of the sample has been recorded. The chemical shift of the hydrogen atom H<sub>28</sub> has been recorded at a value of 8.462 ppm [1] due to the carbon atom C<sub>16</sub>. The H<sub>24</sub> hydrogen atom has a chemical shift of 8.340 ppm. The chemical shifts of hydrogen atoms H<sub>26</sub> and H<sub>27</sub> has been found at the value of 7.261 ppm. The chemical shift of H<sub>22</sub> and H<sub>23</sub> has been found to be 8.928 ppm and 8.908 ppm respectively. The chemical shift of C<sub>5</sub> and C<sub>3</sub> carbon atoms has been found to be 158.77 ppm. The C<sub>1</sub> carbon atom has a chemical shift of about 141.37 ppm. The hydrogen atom H<sub>25</sub> has a chemical shift of about 8.477 ppm. The Chemical shift of the C<sub>13</sub> and C<sub>15</sub> carbon atoms has been recorded to be 111.43 ppm.

**Keywords:** FTIR; FT-Raman; UV-Vis; NMR; Chemical Shift

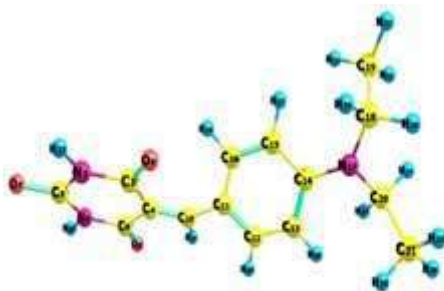


Fig. Atom numbering scheme of DBT

## **The ionic conductivity of bio-polymer poly vinyl alcohol with Indian medicinal plants – Acalypa indica and potato extract for electrochemical devices application**

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### **Abstract**

Bio-polymer electrolyte Polyvinyl alcohol (PVA) with Acalypa indica (Kuppameni leaves) & Potato extract used as solvent and prepare polymer electrolyte by solution-casting technique. The increase in amorphous nature of the bio-polymer electrolyte due to the medicinal plants Acalypa indica and Potato extract has been confirmed by X-ray diffraction analysis. From the complex formation between the polymer and medicinal plants has been confirmed by Fourier transform infra-red spectroscopy. From the AC impedance spectroscopic analysis, the ionic conductivity value has been found to be  $1.5 \times 10^{-4}$  S/cm at ambient temperature for the composition of 1.0 g PA with 100ml of Acalypa indica and potato extract. The dielectric behavior and modulus spectra have been analyzed using AC impedance spectra and the relaxation frequency ( $\tau$ ) has been calculated from the loss tangent spectra ( $\tan \delta$ ).



## Triggering of white light emission from Dy<sup>3+</sup> doped LaAlO<sub>3</sub> nanophosphors by co-doping with Bi<sup>3+</sup> ions for white LED applications

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### Abstract

Bi and Dy co-doped LaAlO<sub>3</sub> nanophosphors were prepared using the Polyol technique to study increased photoluminescence. PXRD and Photoluminescence characterizations were used to investigate the structure and luminescence studies of the nanophosphors. It was found that Dy<sup>3+</sup> ions had an outstanding characteristic emission at 576nm with an increase in photoluminescence during the <sup>4</sup>F<sub>9/2</sub>-<sup>6</sup>H<sub>13/2</sub> transition when compared with single doping and co-doping with Bi<sup>3+</sup>. The Commission International De l'Eclairage (CIE) graph shows a change in colour coordinates from deep blue to yellowish white light indicates that the developed (LaAlO<sub>3</sub>: Bi<sup>3+</sup>, Dy<sup>3+</sup>) phosphor can be used for single phase material for white LED applications.

**Key Words:** Polyol method, Bismuth co-doping, Photoluminescence, Energy transfer



## Magneto-dielectric response in TbMnO<sub>3</sub> at Room Temperature

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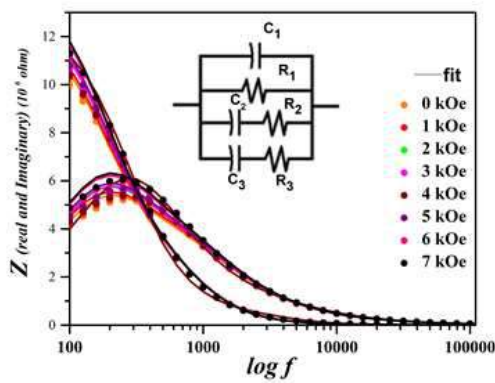
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\*\* Corresponding author: Mail id: [cvunom@hotmail.com](mailto:cvunom@hotmail.com)

### Abstract

TbMnO<sub>3</sub> is a well-known multiferroic material whose magnetic ordering can be controlled by external field and vice versa. This property makes multiferroic material as a potential candidate for memory storage, sensing and spintronics device applications. The highlight in TbMnO<sub>3</sub> is the magnetic interaction is dominated by super-exchange interaction between Mn<sup>3+</sup>-O<sup>2-</sup>-Mn<sup>3+</sup> ions which is governed by Good enough - Kanamori - Anderson rule (GKA).

The current study is focused on the preparation of a phase pure TbMnO<sub>3</sub> by ball milling assisted sintering process and to study its structural and magneto-dielectric property. Phase purity has been confirmed by X – ray diffraction (XRD) and SAED pattern obtained from HR-TEM. Magneto-dielectric study at room temperature on the prepared TbMnO<sub>3</sub>, show variation in dielectric response with respect to the applied magnetic field. The dielectric response is discussed based on the exchange interaction between 4*f* orbital of Tb ion and 3*d* orbital of Mn through oxygen (2*p*). The *Z*" vs log *f* (imaginary part) and dielectric loss (tan δ) spectra strongly reassert the exchange interaction between Mn<sup>3+</sup>-O<sup>2-</sup>-Mn<sup>3+</sup>, affected by Tb<sup>3+</sup>-Tb<sup>3+</sup> and Tb<sup>3+</sup>-Mn<sup>3+</sup> interactions.



The above figure shows impedance spectra (*Z*' and *Z*'') plot as a function of magnetic field, which is fitted by equivalent circuit model of R and C network.

## Molecular Interaction Studies

**R Ajomia and Bharath Kumar\***

*Dr. M.G.R. Education and Research Institute University*

### **Abstract:**

Chemical Industry is the most diversified industrial sectors which include basic chemicals and their derivatives, Petro chemicals, fertilizers, paints, pharmaceuticals, dyes, detergents, pesticides, synthetic rubber, paper etc. Liquids, Liquid mixtures and solution have found wide applications in Chemical, Textile, Leather and Nuclear Industries. Measurement of Ultrasonic velocity, density and viscosity are used to study various types of Molecular interactions that exist in liquid mixtures. Study of Acoustical parameters, Excess thermodynamic functions and theoretical models are useful in determining the nature and strength of the interactions. In the present investigation ultrasonic velocities have been measured in liquid mixtures to understand molecular interactions and various models are employed to calculate the velocities. Excess thermodynamic parameters have been determined. Stability constant for the mixtures is also calculated. The results are tabulated and discussed, for a number of binary liquid mixtures, which include bio - active liquids. Scaled Particle Theory is applied to find the partition function.



## **The characterization of unidirectional and woven Palm fiber, Cane fiber, Sun grass reinforced with epoxy resin composites**

Syed Azfarul Haque<sup>1</sup>, Bipin Kumar Chourasia<sup>2</sup>, Ishita Ghosh<sup>1</sup>, M.K. Paswan<sup>2</sup>

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*2 Department of Mechanical Engineering, National Institute of Technology, Jamshedpur*

### **Abstract**

The climate change led to several problems such as ecosystem, irrigation, and sedimentation. The rapid growth of water natural rivers, lake and canals causes drainage problems in many nations. As a result, the environment is lack of oxygen so we need to grow big plants like Palm tree, bamboo tree, Cane plant which are easily plated and lack of care and are taking small areas so it can grow in anywhere such as in small graden, in sides of roads and in parks and are very useful for the local people as well as for good income source for its fruit we will make palm oil and its wood is also very useful for making ply. Same as cane plants are also very useful for light furniture industries, i have an idea to use these plant fiber make by the the applying composite material method with the use of epoxy and hardner to make natural fiber which is very demanding in industrial application such as bullet proof jacket, vehicle body and light weight application. As in Jharkhand the state is rich of good quality of soil if we grow plants for major industrial application it will support to rise the nationl income and state income and it creat jobs for the local peoples too. This study investigated the development and use of plant fiber for the production of unidirectional weaved fiber epoxy resin composites. The purpose of this research is to investigate at the mechanical and physical properties of unidirectional and woven fiber reinforced epoxy resin composites in variation is (Palm 170gm., sun grass 150gm., palm fiber 60gm) in weight 10: 3 epoxy and hardener mixed. The composites were manufactured through the hand lay-up method. The tensile and impact tests were carried out based on ASTM D3039 and the results of this study showed that increasing of % wt. of the palm fiber, the tensile strength of composite decrease.

***Keywords- Palm Fiber, Cane fiber and Sun Grass fiber, hand lay-up, mechanical properties, epoxy and hardener***









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