

amal nathan <nathan.amalphysics@gmail.com>

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## UGC-DAE CSR \*\* CRS Project (2022-23)Status\*\*

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**UGC-DAE CSR** <support@csruserportal.com>  
Reply-To: support@csruserportal.com  
To: nathan.amalphysics@gmail.com

Wed, May 24, 2023 at 12:02 AM

### Welcome to UGC-DAE CSR

Dear Dr. Dr.M.Amalanathan,

The updated status of your CRS project can now be seen at our user portal. Due to the limited amount of funds received from UGC, funds could be released only to some CRS projects. It is anticipated that funds for remaining CRS projects will soon be available from UGC and subsequently released. Please login to your account to view the sanction order and status of your project.

With best regards,

User Office, UGC-DAE CSR

Note: This is a system generated email. Please don't reply.

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CRS/2022-23/01/662



Accepted

No

Yes

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## CRS project approved without student fellowship

Inbox ×

CRS Project <support@csruserportal.com>  
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UGC-DAE Consortium for Scientific Research  
(An Autonomous Institution of University Grants Commission, New Delhi)

## CRS Program

## CRS Projects FY 2022-23.

Dear Dr.M.Amalanathan,

With reference to the CRS project proposal **CRS/2022-23/804** submitted at L evaluated by the User Committee and the status of your project proposal is:**Approved without student fellowship.**

Kindly note that we have received a larger number of project proposals and due only few could be approved with a student fellowship.

In case you are willing to take up this project, please login to our user port **March 25, 2023**. Guidelines: [https://www.csruserportal.com/data/Guidelines\\_for\\_Project\\_Proposals.pdf](https://www.csruserportal.com/data/Guidelines_for_Project_Proposals.pdf)

Please note that the decision of the User Committee is final and no comm



CRS/2022-23/804

## Chosen Centre: Indore

<b>Project details</b>	
Project title:	Synthesis of noble metal doped/transition metal oxide nanostructured composite for super capacitor electrode
Type of Project:	In-house facilities of Indore Centre
Name(s) of Principal Collaborator from UGC-DAE CSR:	Dr. R. Venkatesh
Names(s) of other Collaborator(s) from UGC-DAE CSR (if any):	N.P. Lalla
Names(s) of Collaborators from DAE (if any):	Rajamani Raghunathan
Is there an ongoing CRS project of UGC-DAE CSR as a PI?	No
Financial support required from UGC-DAE CSR?	Yes
Require Fellowship for a Student?	Yes
Consumable (MAX 50,000/- PER YEAR):	Yes
contingency (MAX 15,000/- PER YEAR):	Yes
Do you have any ongoing/submitted project with SERB/UGC/CSIR/BRNS or other funding agencies?	No
<b>Personal Information</b>	
Name of the Principal Investigator (PI):	Dr.M.Amalanathan
Date of Birth:	1984-03-09
Designation:	Head of the Department
Affiliation:	Nanjil Catholic College of Arts and Science
Official E-mail address:	nathan.amalphysics@gmail.com
Postal address:	Nanjil Catholic College of Arts and Science Nedumcodu Kaliyakkavilai Kanyakumari District Pincode: 629153
<b>Bank Details</b>	
Beneficiary Name	Nanjil Catholic College of Arts and Science
Account Number	10270100217857
Bank Name	FEDERAL BANK
IFSC Code	FDRL0001027
Branch Name	PARASALA
<b>Finance Authorities</b>	
Account Officer's Name	Dr.N.R.Sheela
Account Officer's Email	nanjilccas@gmail.com

## **Synthesis of noble metal doped/ transition metal oxide nanostructured composite for super capacitor electrode**

### **1. Introduction**

Energy is one of the major resources used by the humans. Energy consumption has consistently grown in all sectors, including agricultural, industrial, commercial, and residential, during the last few decades, and is anticipated to continue to rise. India has been addressing the effects of energy on the environment, including air, water, land, and waste. In India, the energy industry is essential for both achieving sustainable development goals and minimising environmental externalities. A major issue is reducing the negative impact of air pollution on human health. India's coal supply has increased substantially, and coal continues to be the country's principal energy and power generating source. In the face of tighter air pollution restrictions, new coal power plants that are more efficient, flexible, and release less pollutants will be better positioned for economic viability. An efficient coal sector is critical not just for electricity generation, but also for industrial development in industries such as steel, cement, and fertilisers. Coal is used for power generation, oil is used for transportation and industry, and biomass is used for home heating and cooking. Bioenergy and the majority of coal is generated in the nation. Bioenergy supply has grown slowly in comparison to the explosive expansion of fossil fuels. Hydropower supply has remained reasonably constant over the last decade, growing at a rate of approximately 10%. Wind and solar, on the other hand, have grown at a quick pace, although from considerably lower levels.

Although funding for Nanotechnology has risen dramatically in the last five years, practical application of the research to tackle issues across the studies disciplines remains a challenge. These studies have helped solar cells and fuel cells, but the implications are not represented in today's products. Thin-film nanotechnology, and electrode for batteries are crucial areas for green-cell-based innovations. In the fields of fuel cells, reformers, and hydrogen storage, a number of institutions and research groups are active. The automobile industry will transition to fuel cells, but they must make the best decision for their individual applications. Additionally, cost reduction and dependability can only be achieved through nanotech enabled solutions, which opens up a new market and adds a new dimension to this sector. We've also targeted emerging countries as a market. Portable Nano-enabled fuel cells would be used in the electronics sector. Researchers are currently concentrating their efforts on developing solar PV, lithium batteries, and solar charging infrastructure. The world has witnessed massive research and development in the field of nanotechnology, but the application of the findings in green energy is an area that has yet to be successfully implemented for a variety of reasons, both known and unknown.

This research investigates the current issues in solar and fuel cell energy and suggests nanotechnology-based solutions. We have detailed the current development in this field as well as our previous work in this proposal. Metal embedded metal oxide composite based electrode, for super capacitor application are set to be considerably more helpful than their present counterparts. In this novel work we focused on the consequences of introducing Nano-enabled green cells. In this present work, gives a details report about production, modelling, reliable, high efficient, and low cost, metal embedded metal oxide composite for energy application.

### **2. Objective**

- To fabricate metal doped metal oxide composite nanostructure for super capacitor electrode by hydrothermal method.
- Different nanostructured composites can be synthesized by varying dopant and synthesis parameters.
- Structural, optical, morphological and electrochemical properties are to be carried out using analytic instruments.
- Tuning the band gap and electrochemical behaviour by varying oxygen stoichiometry in the metal oxides, heat treatment, inclusion of dopant, fabricate suitable nanostructured composite.
- To commercialize the nanostructured composite as a super capacitor electrode.

#### **4. Novelty of the research**

- Tailoring the properties of electrode: tuning the band gap by oxygen stoichiometry in the metal oxide, by adding dopant.
- To enhance the surface area of the electrode by inclusion of co-catalyst.
- By encapsulating noble metal doped metal oxides increases the capacitance value and stability.
- Different nanostructure of metal oxides is to be synthesized and the structure- property reaction will be studied.

#### **4. Methodology**

High quality noble metal doped metal oxide composite will be synthesized by hydrothermal techniques and the properties will be tailored using various parameters and different annealing temperature.

## NAME: M.AMALANATHAN

### Objectives:

To pursue a career with leading corporate of hi-tech environment with committed and dedicated people, which will help me to explore myself fully and realize my potential



### Email:

[nathan.amalphysics@gmail.com](mailto:nathan.amalphysics@gmail.com)  
[nathan.amalphysics2011@gmail.com](mailto:nathan.amalphysics2011@gmail.com)

### Address for Communication: -

**M.Amalanathan**  
**S/O. J.Michael**  
**East kalpahaseri vilai**  
**Vavarai**  
**S.T.Mankad (Post)**  
**Kanniyakumari district**  
**Tamil nadu**  
**Pin : 629172**

**Ph : 04651-293178**  
**Mob : 9940347178**  
**: 7598864911**

### Personal Data

**Date of Birth : 09-03-1984**

**Age : 38**

**Sex : Male**

**Nationality : Indian**

**Community : BC**

**Religion : RC Christian**

### Education:

- **Ph.D Physics (University of Kerala) (Regular)**
- **M.Phil Physics (St.Joseph's college,Trichy) (Regular)**
- **M.Sc Physics (St.Joseph's college,Trichy) (Regular)**
- **B.Sc Physics (Annai velankanni college,Tholayavattam)**
- **H.Sc (St.Francis H.S.S, Vavarai)**
- **S.S.L.C (St.Francis H.S.S, Vavarai)**

### Published Papers:

- ❖ **Published 57 papers in International Journals**
- ❖ **Published 3 papers in National Journals**
- ❖ **Communicated 3 papers in International Journals**
- ❖ **Presented and Participated in 17 National and International Seminars/Conference**

### Languages known:

- **Tamil (Reading, Writing, Speaking)**
- **English (Reading, Writing, Speaking)**
- **Malayalam (Speaking)**

### Award Received:

- ❖ **Dr. APJ Abdul Kalam Award for Scientific Excellence - 2016**

### Research Experience:

- **Reviewer in Spectrochimic Acta, Journal of Molecular Structure, Canadian Journal of Physics, Journal of Theoretical and Computational Chemist**
- **Two years working in UGC Major Project as a project assistant**
- **Organized Three National seminar**
- **Guided 4, Guiding 4 Ph.D Students and Guided 10 M.Phil Student**

### Other Experience:

- ❖ **Research Guide in Manonmaniam Sundaranar University**
- ❖ **IQAC Co-ordinator and Assistant coordinator**
- ❖ **Staff association secretary 2 years**
- ❖ **Chief Superintendent and Additional Chief Superintendent**
- ❖ **Membership in Asian Journal of Physics**
- ❖ **Head in the Department of Physics, Nanjil Catholic College of Arts and Science**
- ❖ **Edited 2 ISBN books**

### Academic profile

Courses	Name of the Institution	Year of Passing	Board/University	Marks Obtained	Maximum Marks	Percentage	Class
Ph.D	Mar Ivanios College Thiruvananthapuram	June 2012	University of Kerala	-	-	-	-
M.phil., Physics	St.Joseph's college (Autonomous), Trichy	Aug 2007	Bharathidasan University	313	400	82.80	I
M.Sc., Physics	St.Joseph's college (Autonomous), Trichy	April 2006	Bharathidasan University	1253	1700	68.7	I
B.Sc., Physics	Annai Velankanni college, Tholayavattam	Apr. 2004	Manonmanium Sundharanar University	1328	2000	66.4	I
H.Sc.,	St.Francis H.S.S., Vavarai	Apr. 2001	State Board	739	1200	61.58	I
S.S.L.C.,	St.Francis H.S.S., Vavarai	Apr. 1999	State Board	343	500	68.6	I

### Teaching Experience

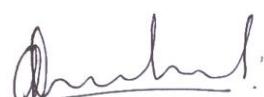
Sl.No	Name of the Institution	Period		Nature of Employment			Total Years
		From	To	Mode of Institution	Mode of Appointment	Teaching level	
1	Annai Velankanni College, Tholayavattam	13-07-2011	15-12-2016	Self-Finance	Regular	UG, PG, & M.Phil	5 Years 5 Months
2	Nanjal Catholic College of Arts and Science, Kaliyakkavilai	15-12-2016	Till Date	Self-Finance	Regular	UG, PG, M.Phil & Ph.D	4 Years 4 Months

### Declaration

I here by declare that the above statements are true, complete and correct to the best of my knowledge and belief

Place: Vavarai

Yours Sincerely



(M. Amalanathan)

Date: 14-10-2022

## ` List of Publication

### **List of International Publication:**

1. **Theoretical and vibrational spectral investigation of sodium salt of Acenocoumarol**  
Hubert Joe, Irena Kostova, C. Ravikumar, **M. Amalanathan** and S. Cinta Pinzaru  
**Journal of Raman Spectroscopy 40 (2009) 1033-1038. (ISSN: 1097-4555)**
2. **NBO analysis and vibrational spectra of 2,6-bis(p-methyl benzylidene cyclohexanone) using density functional theory**  
L. Padmaja, **M. Amalanathan**, C. Ravikumar and I. Hubert Joe  
**Spectrochimica Acta Part A: 74 (2009) 349. (ISSN: 1386-1425)**
3. **Charge Transfer Interaction and Terahertz Studies of a Nonlinear Optical Material L-Glutamine Picrate: A DFT Study**  
**M. Amalanathan, I. Hubert Joe and S.S. Prabhu**  
**Journal of Physical Chemistry A 114 (2010) 13055–13064. (ISSN: 1089-5639)**
4. **Density functional theory calculation and vibrational spectral analysis of 4-hydroxy-3-(3-oxo-1-phenylbutyl)-2H-1-benzopyran-2-one**  
**M. Amalanathan, I. Hubert Joe and Irena Kostova**  
**Journal of Raman Spectroscopy 41(2010) 1076–1084. (ISSN: 1097-4555)**
5. **Molecular first order hyperpolarizability and vibrational spectral investigation of Warfarin Sodium**  
Irena Kostova, **M. Amalanathan** and I. Hubert Joe  
**Chemical Physics 78 (2010) 88–102. (ISSN: 0301-0104)**
6. **Infrared and Raman spectra, vibrational assignment, NBO analysis and DFT calculations of 6-aminoflavone**  
Y. Erdogan, O. Unsalan, **M. Amalanathan** and I. Hubert Joe  
**Journal of Molecular Structure 980 (2010) 24-30. (ISSN: 0022-2860)**
7. **Molecular structure, vibrational spectra and nonlinear optical properties of L-Valine Hydrobromide: DFT study**  
**M. Amalanathan, I. Hubert Joe and V.K. Rastogi**  
**Journal of Molecular Structure 985 (2011) 48-56. (ISSN: 0022-2860)**

**8. Vibrational and Terahertz spectral Investigation and nonlinear optical properties of L-Phenylalanine phenylalanium nitrate -A DFT study**

**M. Amalanathan, I. Hubert Joe and V.K. Rastogi**

**Journal of Molecular Structure 1006 (2011) 513-526 . (ISSN: 0022-2860)**

**9. Density functional theory calculations and Vibrational spectral analysis of 3,5-(Dinitro benzoic acid)**

**M. Amalanathan, I. Hubert Joe, M.A. Palafox, Satentra kumar, V.K. Rastogi**

**Spectrochimica Acta A 78 (2011) 437-1444. (ISSN: 1386-1425)**

**10. Intramolecular charge delocalization and nonlinear optical properties of push- pull chromophore 1-(4-N, N-dimethylaminopyridinium) acetic acid bromide monohydrate from vibrational spectra**

**C. Jesintha John, M. Amalanathan, D.Sajan , K. Udaya Lakshmi and I. Hubert Joe**

**Spectrochimica Acta A78 (2011) 264-272. (ISSN: 1386-1425)**

**11. Vibrational spectra and first order hyperpolarizability studies of Dimethyl amino pyridinium 4-nitrophenolate 4-nitrophenol**

**C. Jesintha John, M. Amalanathan, A.R.Twinkle, P. Srinivasan and I. Hubert Joe**

**Spectrochimica Acta Part A 81 (2011) 151-161. (ISSN: 1386-1425)**

**12. Analysis of Vibrational Spectra and Nonlinear Optical Properties of Organic Molecule L-Alaninium Formate**

**C. Jesintha John, T.S. Xavier, M. Amalanathan, I. Hubert Joe and V.K. Rastogi**

**Spectrochimica Acta Part A 86 (2011) 174-180. (ISSN: 1386-1425)**

**13. Vibrational spectral analysis of nonlinear optical crystal L-Prolinium picrate: A density functional theory study**

**Bismi Edwin, M. Amalanathan and I. Hubert Joe**

**Spectrochimica Acta 96 (2012) 10-17. (ISSN: 1386-1425)**

**14. Vibrational Spectral Investigation and Natural Bond Orbital analysis of anti-Rheumatoid drug Ethyl 4-nitrophenylacetate - DFT approach**

**D.M. Suresh, M. Amalanathan, S. Sebastian, D. Sajan, I. Hubert Joe, V. Bena Jothy**

**Spectrochimica Acta (2012) 98 (2012) 413-422. (ISSN: 1386-1425)**

**15. Molecular structure, Normal Coordinate Analysis, Harmonic Vibrational frequencies, Natural Bond Orbital, TD-DFT calculations and biological activity analysis of antioxidant drug 7-hydroxycoumarin**

S. Sebastian, S. Sylvestre, D. Jayarajan, **M. Amalanathan**, K. Odayakumar, T. Gnanapoongothai, T. Jayavarthan

**Spectrochimica Acta 101 (2013) 370-381. (ISSN: 1386-1425)**

**16. FT-IR, FT-Raman, FT-NMR spectra and DFT simulations of 4-(4-Fluoro-phenyl)-1H-imidazole**

Y. Erdogan, D. Manimaran, **M. Amalanathan** and I. Hubert Joe  
**Optics and Spectroscopy, 114, 2013, 525–536. (ISSN: 1562-6911)**

**17. Vibrational spectral investigation and molecular polarizability studies of NLO crystal Naphthalene Picrate for THZ application**

**M. Amalanathan**, V.K. Rastogi and I. Hubert Joe  
**Spectrochimica Acta 108, 2013, 256-267. (ISSN: 1386-1425)**

**18. Vibrational Spectra, Molecular Structure, Natural Bond Orbital, First Order Hyperpolarizability, TD-DFT and Thermodynamic analysis of 4-amino-3-hydroxy-1-naphthalenesulfonic acid by DFT approach**

S. Sebastian, S. Sylvestre, N. Sundaraganesan, **M. Amalanathan**, S. Ayyapan, K. Odayakumar, B. Karthikeyan  
**Spectrochimica Acta 107(2013) 167-178. (ISSN: 1386-1425)**

**19. Vibrational Spectral Investigation and natural bond orbital analysis of Pharmaceutical compound 7-Amino-2,4-dimethylquinolinium formate- DFT approach**

D.M.Suresh, **M. Amalanathan**, S. Sebastian, D.Sajan, I. Hubert Joe and V.Bena Jothy, Ivan Nemec  
**Spectrochimica Acta 115 (2013) 595-602. (ISSN: 1386-1425)**

**20. Normal coordinate analysis and Nonlinear Optical Response of cross-conjugated system 4,4-Dimethyl Benzophenone**

**M. Amalanathan**, T.S. Xavier, I. Hubert Joe and V.K. Rastogi  
**Spectrochimica Acta 116 (2013) 574-83. (ISSN: 1386-1425)**

**21. Molecular structure, vibrational spectral investigation and the confirmation analysis of 4-Methylesculetin molecule**

Y. Erdogan, M. Guzel, M. T. Güllüoğlu, **M. Amalanathan**, S. Saglam, I. Hubert Joe  
**Optics and Spectroscopy, 116, 2013, 348–359. (ISSN: 1562-6911)**

**22. Studies on molecular structure, vibrational spectra and molecular Docking analysis**

**of 3-Methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl 4-aminobenzoate**

D.M.Suresh , **M. Amalanathan**, I. Hubert Joe, V.Bena Jothy , and Yun-Peng Diao

**Spectrochimica Acta 130( 2014) 591-603. (ISSN: 1386-1425)**

**23. Vibrational Spectra (FT-IR and FT-Raman), Molecular Structure, Natural Bond Orbital, and TD-DFT analysis of L-Asparagine Monohydrate by Density Functional Theory approach**

S. Sylvestre, S. Sebastian, S. Edwin, **M. Amalanathan**, S. Ayyapan, T. Jayavarthanam, K. Odayakumar, S. Solomon

**Spectrochimica Acta 133 (2014) 190-200. (ISSN: 1386-1425)**

**24. Study on conformational stability, molecular structure, vibrational spectra, NBO, TD-DFT, HOMO and LUMO analysis of 3,5-dinitrosalicylic acid by DFT techniques**

S. Sebastian, S. Sylvestre, J. Jayabharathi, S. Ayyapan, **M. Amalanathan**, K. Odayakumar, Ignatius A. Herman

**Spectrochimica Acta 136 (2015) 1107-1118. (ISSN: 1386-1425)**

**25. FT-IR and FT-Raman spectral investigation and DFT Computations of Pharmaceutical Important Molecule: Ethyl 2-(4-Benzoyl-2,5-Dimethylphenoxy) Acetate**

D.M.Suresh, **M. Amalanathan**, I. Hubert Joe, V.Bena Jothy , S.Sebastian and S.Ayyapan **Pharmaceutica Analytica Acta 7 (2016) 1-9 (ISSN: 2153-2435)**

**26. FT-IR Molecular structure and Charge transfer contributions to nonlinear optical property of 2-Methyl-4-Nitroaniline: A DFT Study**

G.Femina Jasmine, **M. Amalanathan**, S.Dawn Dharma Roy

**Journal of Molecular Structure 1112 (2016) 63-70. (ISSN: 0022-2860)**

**27. Infrared Spectral Investigations and Ab Initio Computations of Pharmacological Drug Goniofufurone Monoacetate**

**Amalanathan M**, Usha D, Hubert Joe I and Ajithabai MD

**Pharmaceutica Analytica Acta 7:8 (2016) 1-7(ISSN: 2153-2435)**

**28. Comparative studies on Molecular structure, Vibrational Spectra and Hyperpolarizabilities of NLO Chromophore Ethyl 4-Dimethylaminobenzoate**

**M. Amalanathan**, Femina Jasmine, S.Dawn Dharma Roy

**Journal of Molecular Structure 1141 ( 2017) 400-416. (ISSN: 0022-2860)**

**29. Structure activity relationship, vibrational spectral investigation and molecular docking analysis of anti-neuronal drug 4-(2-Aminoethyl) Morpholine**

Bismi Edwin, **M. Amalanathan**, Ridhima Chadha, Nandita Maiti, Sudhir Kapoor and I. Hubert Joe

**Journal of Molecular Structure 1148 (2017) 459-470. (ISSN: 0022-2860)**

**30. Quantum chemical computations on structural elucidation, homo-lumo and NLO analysis of 5-chloro-2-hydroxypyridine**

D.Usha , **M. Amalanathan**, H.Marshan Robert

**International Journal of Engineering Science and Innovative Technology (IJESIT)**  
7( 2018) 67-75 (ISSN: 2319-5967)

**31. FT-Raman and FTIR Spectroscopic Investigation, First Hyper Polarizability, Homo**

**Lumo Analysis of P-Fluorobenzonitrile (PFBN)**

S. Aslin, D. Usha, **M. Amalanathan**

**International Journal of Science and Research (IJSR) 7, 2018, 1144-1149 (ISSN: 2319-7064)**

**32. Identification of Anticoagulants Activity using Structural, Spectroscopic and Molecular Docking Analysis of 6-Methyl Coumarin**

Loice Bessylet, C.Gnana Sambandam, **M. Amalanathan** and D.Usha

**International Journal of Research and Analytical Reviews (IJRAR) 5, 2018, 652-665 (E-ISSN 2348-1269, P- ISSN 2349-5138)**

**33. Terahertz studies of some nonlinear optical material**

**M. Amalanathan** and D.Usha

**International Journal of Research and Analytical Reviews (IJRAR) 5, 2018, 399-407 (E-ISSN 2348-1269, P- ISSN 2349-5138)**

**34. Identification and Analysis of anticancer and antimicrobial activity of 1-(p-toluenesulfonyl)imidazole using theoretical and experimental analysis**

G. Golding Sheeba , D. Usha, **M. Amalanathan** , and M. Sony Michael Mary

Journal of Theoretical and Experimental Biology, 13 (1 and 2): 111-123, 2018 (ISSN: 0972-9720)

**35. Structural Analysis, Vibrational Spectral Investigation and Charge Transfer Interactions of 5-ChloroSalicylaldehyde by Experimental and Theoretical Investigations**

B. Queen Sheeba, C. Besky Job, M. Sony Michael Mary, **M. Amalanathan**, R. Racil Jeya Geetha

**Journal of Theoretical and Experimental Biology 13 (1 and 2): 125-134, 2018,  
(ISSN: 0972-9720)**

**36. Moleculr Docking, Harshiefield Surface And Reactivity And Hyperpolarizability**

**Analysis Of 3-(2-Bromoacetyl)-2h-Chromen-2-One**

S.Loice Bessylet, C.Gnana Sampantham, **M.Amalanathan**, D.Usha and M.Sony

Michael Mary **Journal of Emerging Technologies and Innovative Research 6, 2019,  
211-225** (ISSN-2349-5162)

**37. Investigations On The Optical And Mechanical Properties Of Non Linear Optical  
Creatininium Phosphite Single Crystal**

Sindhusha S, Padma C M, **Amalanathan M**

**International Journal of Scientific & Technology Research 8, 2019, 1676-1682**  
(ISSN 2277-8616)

**38. Spectroscopic (UV, NMR) Investigation, Anti- Microbial And Molecular Docking  
Analysis Of 2,3- Dichloronaphthalene-1,4-Dione**

Marshan Robert H, **Amalanathan M**, Usha D, Racil Jeya Geetha R, Sony Michael Mary  
M

**International Journal of Scientific & Technology Research 8, 2019, 2127-2134**  
(ISSN 2277-8616)

**39. Vibrational spectral, density functional theory and molecular docking analysis on  
4-nitrobenzohydrazide**

H. Marshan Robert , D Usha , M. Amalanathan , R. Racil Jeya Geetha d, M. Sony Michael Mary

**Journal of Molecular Structure 1223 (2020) 128948 (ISSN: 0022-2860).**

**40. Vibrational Spectroscopic Analysis of 10H-Dibenzo[b,e][2,4]oxazine and nvestigate  
their Structural Reactivity by DFT Computations and Molecular Docking Analysis**

M. Latha Beatrice, S. Mary Delphine, M. Amalanathan And H. Marshan Robert

**Asian Journal of Chemistry; Vol. 32, No. 10 (2020), 2475-2485 (ISSN: 0970-7077)**

**41. Structural, morphological, and optical properties of country egg shell derived  
activated carbon for dye removal**

M. Aravind, **M Amalanathan**

**Materials Today: Proceedings Volume 43, Part 2, 2021, Pages 1491-1495 ISSN:  
2214 -7853**

**42. A Spectroscopic (IR, Raman, UV, NMR) Characterization and investigation of  
reactive properties of pyrazine-2-carboxamide by anti-bacterial, anti-  
mycobacterial, fukui function, molecular docking and DFT calculations**

H. MarshanRobert, D.Usha, **M.Amalanathan**, R. Racil JeyaGeetha, M. Sony Michael Mary

**Chemical Data Collections Volume 30, December 2020, 100583 ISSN: 2405-8300**

**43. Identification of structure activity relation of a synthetic drug 2,6-pyridine dicarbonitrile using experimental and theoretical investigation**

G.Golding Sheeba, D.Usha, **M.Amalanathan**, M.Sony Michael Mary

**Wutan Huatan Jisuan Jishu Volume XVI, Issue XI, November/2020 Page:89-113**

**ISSN:1001-1749**

**44. Quantum chemical computation, vibrational analysis, molecular structure, nonlinear optical studies of 4-(Diethylamino)salicylaldehyde**

B.Queen Sheeba, , C. Besky Job, M.Sony Michael Mary, **M.Amalanathan**

**Wutan Huatan Jisuan Jishu Volume XVII, Issue I, January 2021Page:268-295**

**ISSN:1001-1749**

**45. Critical green routing synthesis of silver NPs using jasmine flower extract for biological activities and photocatalytical degradation of methylene blue Author links open overlay panel**

M.Aravind, AwaisAhmad, IkramAhmad, **M.Amalanathan**, KhalidaNaseem, Sony M. MichaelMary, C.Parvathiraja, ShahidHussaingTahan, SaadAlgarnihMuhamma, Pervaiz, Muhamma, Zubair,

**Journal of Environmental Chemical Engineering Available online 9 December 2020, 104877 In Press, ISSN: 2213-3437**

**46. Synthesis of TiO<sub>2</sub> nanoparticles by chemical and green synthesis methods and their multifaceted properties**

M. Aravind M. **Amalanathan1** and M. Sony Michael Mary

**SN Applied Sciences (2021) 3:409**

**47. Molecular Structure, Spectroscopic, Fukui function, RDG, Anti-microbial and Molecular Docking analysis of higher concentration Star Anise content compound Methyl 4-methoxybenzoate -DFT Study**

Latha Beatrice, S.Mary Delphine, **M.Amalanathan**, M.Sony Michael Mary, H.Marshan Robert, K.Thibi Mol

**Journal of Molecular Structure 1238, 2021, 130381**

**48. Spectroscopic Profiling (FT-IR, FT-Raman), Vibrational Assignments, Wave Function (ESP, ELF, LOL) Analyses and Fukui Function Study of NBenzylidene Aniline (NBAN)**

S.Aslin, D.Usha, **M.Amalanathan**

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**49. Molecular Structure, Vibrational Spectroscopic,Frontier Molecular orbital and Natural Bond Orbital analysis of Anti-cancer drug 6-Chloro-3- Pyridine Carbonitrile**

G.Golding Sheeba,b, D.Usha , **M.Amalanathan**, M.Sony Michael Mary, H.MarshanRobert

**Spectroscopy Letters 2021, VOL. 54, No. 6, 419–436**

**50. Structural and vibrational spectral investigation on the identification of Non Linear Optical properties and wave function analyses (Electrostatic potential, Electron localization Function, Localized Orbital Locator) of 3-Ethoxy Salicilaldehyde**

B.Queen Sheeba, M.Sony Michael Mary, **M.Amalanathan**, C. Besky Job  
**Molecular Simulation Vol. 47, 2021, Pages 1217-1233 |**

**51. Enhanced photocatalytic and biological observations of green synthesized Activated carbon, Activated carbon doped Silver and Activated carbon/Silver/Titanium dioxide nanocomposites**

Aravind.M, **Amalanathan. M**, Sony Michael Mary.M, C.Parvathiraja, Asma A. Alothman, Saikh M. Wabaidur, Mohammad Ataul Islam  
**Journal of Inorganic and Organometallic Polymers and Materials 32, (2022) pages267–279.**

**52. Synthesis, Structural, Spectroscopic and Docking Studies on (E)-1-Ferrocenyl-3-phenyl-propen-1-one by Density Functional Theory**

**M.Amalanathan**, M.Sony Michael Mary, M.Latha Beatrice, S.Mary Delphine , H.Marshan Robert, A.R.Twinkle, Zoran Ratkovic, Y.Samson  
**Molecular Simulation Vol. 48, 2022, 387–402**

**53. Synthesis of silver nanoparticles using Syzygium malaccense fruit extract and evaluation of their catalytic activity and antibacterial properties**

Herbin Basalius H, Aravind. **M, Amalanathan** , Sony Michael Mary. M4, Maria Lenin. M, C. Parvathiraja, Masoom Raza Siddiqui, Saikh Mohammad Wabaidur, Md Ataul Islam.

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**54. Synthesis, Structural, Spectroscopic investigation on 3-(2-Hydroxyphenyl)-1-ferrocenylpropan-1-one by Density Functional Theory**

M.Sony Michael Mary, R. Racil Jeya Geetha, **M.Amalanathan**, A.R.Twinkle Zoran Ratkovic

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**55. Structure Activity Relationship, Topological Analysis and Molecular Docking Analysis of Pharmaceutical Molecule 2356 -Tetrafluoro-4-Pyridine Carbonitrile**

M. Sony Michael Mary, R. Racil Jeya Geetha , **M. Amalanathan** and R. Benisha

**Journal of Pharmaceutical Research International 33(60B): 2886-2902, 2021**

**56. Spectroscopic and Topological analysis and in vitro antimicrobial activity of Phenothiazine**

**M.Sony Michael Marya, R. RacilJeya Geetha, M.Amalanathan, H.Marshan Robertd, A.Ronaldo Anuff**

**Spectroscopy Letters 55, 2022 - Issue 3, 212-228**

**57. Catharanthus roseus leaf extract mediated Ag-MgO nanocatalyst for Photocatalytic degradation of congo red dye and their antibacterial activity**

R.Benisha, M.Amalanathan, M.Aravind, M Sony MichelMary, AwaisAhmad, SobiaTabassum, Wahidah H.Al-Qahtani, IkramAhmad

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**58. Green synthesis of nano silver using Syzygium samarangense flower extract for multifaceted applications in biomedical and photocatalytic degradation of Methylene Blue.**

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**Applied Nano Science ( 2022)**

**List of National Publication:**

**1) Density functional theory calculation and vibrational spectroscopic study of p-Hydroxy benzoicacid dimer**

V. Bena Jothy, M Amalanathan, V.K Rastogi, I. Hubert Joe

**Asian Journal of Physics, Vol. 24 (2015) 00-00.**

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**2) Molecular structure and spectroscopic properties of L-Histidinium dihydrogen monophosphate monohydrate: FT-Raman, FT-IR ,SERS and DFT computations**

V. Bena Jothy, M. Amalanathan, V.K. Rastogi and I. Hubert Joe

**Asian journal of spectroscopy (2012) 207-224. (ISSN: 0971-9237)**

**3) Molecular Structure, Vibrational spectra and theoretical studies of Bis Glycyl glycinium Oxalate**

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**Asian journal of spectroscopy 2010 87-105. ((ISSN: 0971-9237)**

## Others:

1. **Spectroscopic, Frontier Orbital's and NBO analysis of 3-Pyridinecarboxylic acid hydrazide - DFT method**  
**H.MarshanRobert , D.Usha, M.Amalanathan**  
**Studies in Indian Place Names (UGC Care) 40, 2020, 1041-1050 (ISSN: 2394-3114)**
  
2. **Structural and Spectral Analysis of Picric Acid 2 Nitroaniline A DFT Approach**  
**G.Bagavathi Sankar , D.Usha, M. Amalanathan**  
**Studies in Indian Place Names (UGC Care) 40, 2020, 1197-1203 (ISSN: 2394-3114)**
  
3. **Structural analysis and electronic transfer investigation of a anticancer drug 2,6-pyridinedicarbonitrile**  
**G.Golding Sheeba, D.Usha1 M.Amalanathan, M.Sony Michael Mary**  
**Studies in Indian Place Names (UGC Care) 40, 2020, 1070-1074 (ISSN: 2394-3114).**

## Special issue Papers

1. **Quantum Chemical computations ans spectral Investigation of 2, 6-Bis (P-Methyl Benzylidene Cyclohexanone) M. Amalanathan, C. Ravikuma, L. Padmaja, V.S. Jayakumar andI. Hubert Joe**  
**American Institute of Physics 978-0-7354-0606-3/08**
  
2. **Growth and vibrational spectroscopic Investigations of NLO crystal Barium Thiourea Chloride M. Meena Kumaii, C. Ravikumar, M. Amalanathan, V. S. Jayakumar andI. Hubert Joe**  
**American Institute of Physics 978-0-7354-0606-3/08**
  
3. **Natural bond orbital analysis and vibrational spectral investigation of 3,5-(dinitro benzoic acid)**  
**Rastogi, V.K., Amalanathan, M., Hubert Joe, I.**  
 (2010) AIP Conference Proceedings 1267 PP. 621 - 622 doi: 10.1063/1.3482712
  
4. **Terahertz and FT-IR spectral analysis of a NLO material L-glutamine picrate: A DFT study**  
**Amalanathan, M., Joe, I.H. (2010) AIP Conference Proceedings 1267 PP. 1192 - 1193 doi: 10.1063/1.3482375**
  
5. **Polariton dispersion of a quantum wire superlattice system**  
**K. S. Joseph Wilson, M. Amalanathan, V. Revathy and S. Maria Lenin**  
**AIP Conf. Proc. 1665, 090037 (2015); <http://dx.doi.org/10.1063/1.4918017>**

## Conference Publication:

1. **DFT Computation on Molecular structure and Vibrational Spectral Investigations of NLO Chromophore 2-Amino-3-Nitro Pyridine**  
**G.Femina Jasmine, M. Amalanathan and S.Dawn Dharma Roy**

**UGC sponsored National seminar on Emerging Trends in Theoretical and Experimental Physics, 8<sup>th</sup> & 9<sup>th</sup> January 2015, Organized by Department of Physics, Sree Ayyappa College for Women, Chunkankadai, (ISBN 978-81-9-2-308-2-4).**

2. Studies on Molecular structure, Vibrational Spectral analysis and Hyperpolarizabilities study of 2-Amino-3-Nitro Pyridine  
G.Femina Jasmine, **M. Amalanathan** and S.Dawn Dharma Roy  
**National Seminar on New Materials and Nanotechnology (NSNMN-2015) 1<sup>th</sup> February 2015 Organized by Department of Science and Department of Electronics and Communication Engineering, Heera College of Engineering and Technology, Thiruvananthapuram.**
3. DFT computation on Molecular Structure & Vibrational Spectral Investigations of NLO Chromophore 2-Methyl-4-Nitro Aniline  
G.Femina Jasmine, **M. Amalanathan** and S.Dawn Dharma Roy  
**UGC Sponsored National Conference on Emerging Trends in Applied Physics (NCETAP-2015) 19<sup>th</sup> & 20<sup>th</sup> February 2015 organized by Department of Physics, Lekshmipuram College of Arts and Science, Neyyoor.**
4. Studies on Molecular structure, Vibrational Spectra and Hyperpolarizabilities of NLO Chromophore Ethyl 4-Dimethylaminobenzoate,  
G.Femina Jasmine, C.Sindhiya, **M. Amalanathan** and S.Dawn Dharma Roy  
**National Conference on Technologically Advanced Materials (NCTAM-2016) on 6<sup>th</sup> September 2016 organized by Department of Physics, Muslim Arts college, Thirivithancode (ISSN:2349-6886).**
5. Nonlinear Optical Response of cross-conjugated system 4,4-Dimethyl Benzophenone **M. Amalanathan, T.S. Xavier, I. Hubert Joe and V.K. Rastogi**  
**National Conference on Exploring the Frontier of Vibrational Spectroscopy (EXFOVIS-2011) (Sept 1-2, 2011) at Women's Christian College .**
6. Charge transfer interaction and vibrational spectral investigation of a nonlinear optical material L-Glutamine Picrate: A DFT study  
**M. Amalanathan and I. Hubert Joe**  
**98th Indian Science congress (ISCA 2011) (Jan 3-7, 2010) at SRM University, Chennai.**
7. Density functional theoretical modeling and HOMO-LUMO energy of p- Hydroxy benzoic acid dimmer  
V. Bena Jothy, **M. Amalanathan** and I. Hubert Joe

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8. Vibrational Spectroscopic studies and Natural Bond Orbital Analysis of non linear push-pull chromophore 1-(4-N, Ndimethylaminopyridinium) acetic acid bromide monohydrat  
C. Jesintha John, **M. Amalanathan** and I. Hubert Joe  
**International Conference on Recent Frontiers in Applied Spectroscopy (ICORFAS-2010) 22nd – 24th September, 2010 at Annamalai University Chithambaram.**
9. Quantum Chemical Methods First order hyperpolarizability study and vibrational spectral investigation of the NLO crystal L-Valine Hydrogen chloride  
A.R. Twinkle, **M. Amalanathan** and I. Hubert Joe  
**International Conference on Recent Frontiers in Applied Spectroscopy (ICORFAS-2010) 22nd – 24th September, 2010 at Annamalai University Chithambaram.**
10. Density functional theory and natural bond orbital of p- Hydroxy benzoic acid dimer  
V. Bena Jothy, **M. Amalanathan** and I. Hubert Joe  
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11. Natural Bond Orbital Analysis and Vibrational Spectral Investigation of 3,5-(Dinitro benzoic acid)  
V.K. Rastogi, **M. Amalanathan** and I. Hubert Joe  
**XXII International Conference on Raman Spectroscopy (ICORS 2010) (August 8 – 13, 2010) at Boston, USA. (Accepted).**
12. Teraertz and FT-IR spectral Analysis of NLO material L-Glutamine Picrate: A DFT study  
**M. Amalanathan** and I. Hubert Joe  
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13. FT-IR analysis and First order hyperpolarizability study of NLO crystal Naphthalene picrate  
**M. Amalanathan** and I. Hubert Joe  
**Ninth DAE-BRNS National Laser Symposium-(NLS-09) (Jan 13-16, 2010) at Bhabha Atomic Research Centre (BARC), Mumbai.**
14. FT-IR spectral investigationa and Natural bond orbital analysis of Naphthalene picrate  
**M. Amalanathan** and I. Hubert Joe  
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15. FT-IR Spectral Investigation and NBO analysis of Nonlinear material L-Proline Picrate  
Bismi Edwin, **M. Amalanathan**, C. Ravikumar and I. Hubert Joe  
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16. Quantum chemical computational hyperpolarizability studies of Cyclohexanone derivatives  
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17. Quantum chemical computations and spectral investigation of 2,6-Bis(p-methyl benzylidene cyclohexanone)  
**M. Amalanathan**, C. Ravikumar, L. Padmaja, V.S. Jayakumar and I. Hubert Joe  
**International conference on perspective in vibrational spectroscopy (ICOPVS2008)(Feb 24-28, 2008) at Mascot Hotel, Trivandrum.**

18. Growth and vibrational spectroscopic investigation of NLO crystal Barium Thiourea Chloride  
M. Meena Kumari, C. Ravikumar, **M. Amalanathan**, V.S. Jayakumar and I. Hubert Joe  
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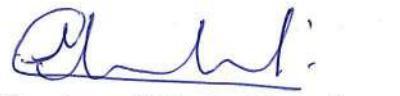
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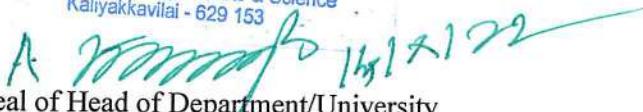
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1. As a Principal Investigator (PI), I understand that it is my responsibility to carry out the Collaborative Research Scheme (CRS) project work as per rules and regulations of UGC-DAE CSR.
2. The scientific program of the CRS will be carried out jointly by me and a Principal Collaborator at UGC-DAE CSR. All scientific publications resulting from the CRS, will be communicated with each other's consent. Technical and scientific assistance from UGC-DAE CSR and DAE personnel will be acknowledged, either in the acknowledgements or in authorship.
3. Financial support received from UGC-DAE CSR will be acknowledged explicitly in all publications. Please add following sentence in the acknowledgement section of the manuscript, **“This work was partially/fully carried out using the facilities of UGC-DAE CSR”**
4. Progress reports, extension requests, conclusion documents, etc., will be submitted by me to the UGC-DAE CSR with the consent of the Principal Collaborator.
5. Copies of the publications, thesis, etc., resulting from the CRS will be sent to UGC-DAE CSR.

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Date:14-10-2022

  
Signature of Principal Investigator  
**DR. M. AMALANATHAN**  
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Sl No.	Abbreviation	Expansion
1	AWB	Any Where Banking
2	CHQ	Cheque
3	Coll.	Collection
4	Comm.	Commission
5	Cr.	Credit
6	DD	Demand Draft
7	Dr.	Debit
8	DW	Dividend Warrant
9	ECS	Electronic Clearing Service
10	FBxxx	Standing Instruction
11	FCCP	Foreign Currency Cheque Purchased
12	IBC	Inward Bills for Collection
13	IBP	Inward Bills under LC
14	ICBP	Inland Clean Bills Purchased
15	IDBP	Inland Documentary Bills Purchased
16	Inst.	Instrument
17	Int.	Interest
18	IO	Interest Outflow
19	LCC	Local Cheque for Collection
20	LCP	Local Cheque Purchased
21	OBG	Outward Bills for Collection
22	Pd.	Paid
23	POS Sur.	Point of Sale Surcharge
24	RTN	Return
25	Tran.	Transaction
26	Trf.	Transfer

B613B

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 Customer ID : 24069359  
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DATE	CHEQUE NO.	PARTICULARS	WITHDRAWALS	DEPOSITS	BALANCE	
तारीख Date	चेक नं. Cheque No.	आवश्यक Particulars	आदाकर Initial	निकासियाँ Withdrawals	जमाएँ Deposits	शेष Balance
30-06-2022	423998	NEFT-CNRB-108AN2		25000.00		964199 Cr
01-07-2022	423999	TO CASH BRUSELIN		8000.00		976199 Cr
01-07-2022	423997	ABRAHAMHOLLOWBRI		150000.00		826199 Cr
3						
4	-07-2022	BY CASH SELF		58650.00		884849.00 Cr
5	-07-2022	SUN SHINE IN		66292.00		818557.00 Cr
6	-07-2022	FATHIMA TRAD		144722.00		673835.00 Cr
7	-07-2022	DHARMARAJ		15300.00		658535.00 Cr
8	-07-2022	Charges for PORD		16.52		658518.48 Cr
9	-07-2022	NEFT-CNRB-10		106720.00		551798.48 Cr
10	-07-2022	AMAL RAJ ELE		38010.00		513788.48 Cr
11	-07-2022	ABRAHAMHOLLO		75000.00		438788.48 Cr
12						
13						
14	-07-2022	MOSES ANAND		58826.00		379962.48 Cr
15	-07-2022	MOSES ANAND		13167.00		366795.48 Cr
16	-07-2022	BENSAM D		100000.00		266795.48 Cr
17	-07-2022	RTGS-FDRL-FDRLH2		500000.00		766795.48 Cr
18	-07-2022	NEFT-IDIB-IDIBH2-101		24500.00		791295.48 Cr
19	-07-2022	INDOSALES KA		28963.00		762332.48 Cr
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