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### **EDUCATION QUALIFICATION**

**Ph.D.**, - Vibrational Spectroscopy; March 2010 – March 2014 Manonmaniam Sundaranar University, Tirunelveli-12, Tamilnadu, India.

**M.Phil.**, - Applied Spectroscopy; April 2004 – September 2006 (**8.75 GP with Distinction**), Annamalai University, Annamalai Nagar, Tamilnadu, India.

**M.Sc.**, - **Physics**; August 2002 – April 2004 (6.75 GP), Annamalai University, Annamalai Nagar, Tamilnadu, India.

**B.Sc.**, - Physics; June 1999 – April 2002 (**66%**), Thanthai Hans Roever College, Perambalur-12, Affiliated with Bharathidasan University, Trichy, Tamilnadu, India.

### **PROFESSIONAL EXPERIENCES: 16.7 Years**

- ❖ Assistant Professor: Department of Physics, SRM University-Ramapuram, Chennai-600089, India (01-07-2013 to till date).
- ❖ Assistant Professor (06-07-2009 to 30-04-2013): PG & Research Department of Physics, Thanthai Hans Roever College, Perambalur, Tamilnadu, India. (06-07-2009 to 30-04-2013)
- ❖ Lecturer : Department of Physics, Muthu Mase Arts & Science College, Harur, Tamilnadu, India. (10.07.2006 to 30.04.2009)

### **LIST OF PUBLICATIONS IN REFEREED JOURNALS (28 papers)**

1. J. Stella Punitha, A. Nataraj, V. Anbarasu, M. Dhilip, M. Manikandan, and K. Saravana Kumar, Influence of La<sup>3+</sup> substitution on the structural, magnetic and electrical characteristics of Sr<sub>2</sub>FeTiO<sub>6</sub> double perovskites, J Mater Sci: Mater Electron (2023) 34:1462, <https://link.springer.com/article/10.1007/s10854-023-10793-0>.

2. Kumar, K.S., Haridharan, N., Ranjith, S., Nataraj, A., Studies on the DFT calculations and molecular docking of versatile molecular sensor 1-(6-Aminopyridin-2-yl) -3-(4-nitrophenyl)

urea, Chemical Physics Impact, 2023, 6, 100139.

<http://dx.doi.org/10.1016/j.chphi.2022.100139>

3. J. Stella Punitha , A. Nataraj , V. Anbarasu , M. Dhilip , M. Manikandan , and K. Saravana Kumar, Influence of La<sup>3+</sup> substitution on the structural, magnetic and electrical characteristics of Sr<sub>2</sub>FeTiO<sub>6</sub> double perovskites, *J Mater Sci: Mater Electron* (2023) 34:1462. <https://doi.org/10.1007/s10854-023-10793-0>

4.K. Anitha; **A. Nataraj**; Badiadka Narayana; T. Karthick, Spectral Characteristics, DFT Exploration, Electronic Properties, Molecular Docking and Biological Activity of 2E-1-(3-Bromothiophene-2-yl)-3-(1, 3-Benzodioxol-5-yl)Prop-2-en-1-One Molecule, *Polycyclic Aromatic Compounds*, 2022-10-02, DOI: [10.1080/10406638.2022.2127802](https://doi.org/10.1080/10406638.2022.2127802)

5. JS Punitha, **A Nataraj**, V Anbarasu, M Dhilip, KS Kumar, Synthesis and characterization of phase-stabilized Gd<sub>2</sub>FeMnO<sub>6</sub> double-Perovskite compound, **Journal of Materials Science: Materials in Electronics**, 32 (8), (2021) 10266-10276.

6. J. Stella Punitha, K. Saravana Kumar, M. Dhilip, V. Anbarasu, and **A. Nataraj**, Characterization of the structural, magnetic and Raman properties of 6f – 4d double perovskite compound, **AIP Conference Proceedings**, 2265, 030526 (2020); <https://doi.org/10.1063/5.0016644>.

7. JS Punitha, M Dhilip, V Anbarasu, **A Nataraj**, KS Kumar, Coexistence of two phases in Sr<sub>2</sub>TiFeO<sub>6</sub> double perovskite, **AIP Conference Proceedings**, 2117 (1), (2019) 020010.

8. K. Anitha, **A. Nataraj**, and B. Narayana, Spectroscopic studies and structural activity investigations of 2E-1-(3-bromothiophene-2-yl)-3-(4-chlorophenyl) prop-2-en-1-one, **AIP Conference Proceedings**, 2117, 020016 (2019); <https://doi.org/10.1063/1.5114596>.

9. **Nataraj A**, T Beena, L Sudha, B Narayana, V Balachandran, Spectroscopic characterization and quantum chemical investigation of molecular structure and vibrational spectra of phthalazine-1 (2H)-one, **Indian Journal of Pure & Applied Physics (IJPAP)** 56 (10), (2018) 802-813.

10. V. Raja, G. Selvan, **A. Nataraj** & R. Anbarasu, Dentification of hazardous minerals in respirable Dust samples in and around ariyalur district in Tamilnadu, **International Journal of Scientific Research and Modern Education (IJSRME)**, 2455 – 5630, Volume 2, Issue 1, 2017.

11. T. Beena, L. Sudha, **A. Nataraj**, V. Balachandran, D. Kannan, M. N. Ponnuswamy, Synthesis, spectroscopic, dielectric, molecular docking and DFT studies of (3E)-3-(4-methylbenzylidene)-

3,4-dihydro-2H-chromen-2-one: an anticancer agent, **Chemistry Central Journal**, **11:6 (2017)**  
DOI 10.1186/s13065-016-0230-8.

12. R. Kavipriya, Helen P. Kavitha, B. Karthikeyan, **A. Nataraj**, Molecular structure, spectroscopic (FT-IR, FT-Raman), NBO analysis of N,N'-diphenyl-6-piperidin-1-yl-[1,3,5]-triazine-2,4-diamine, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, **150 (2015) 476-487**.

13. V. Balachandran, M. Murugan, **A. Nataraj**, M.Karnan, G. Ilango, Comparative vibrational spectroscopic studies, HOMO–LUMO, NBO analyses and thermodynamic functions of p-cresol and 2-methyl-p-cresol based on DFT calculations, **Spectrochimica Acta Part A**, **132 (2014) 538 – 549**.

14. B. Revathi, **A. Nataraj** , V. Balachandran, Quantum Chemical determination of Molecular geometries, Interpretation of FT-IR, FT-Raman spectra and Charge transfer properties for N-(2-Cyanoethyl)-N-methylaniline, **Spectrochimica Acta Part A**, **124(2014)1-11**.

15. V. Balachandran, A. Janaki, **A. Nataraj**, Theoretical Investigations on Molecular Structure, Vibrational spectra, HOMO,LUMO, NBO analysis and hyperpolarizability calculations of thiophene-2-carbohydrazide, **Spectrochimica Acta Part A**, **118(2014)321-330**.

16. M. Karnan, V. Balachandran, M. Murugan, M.K. Murali, **A. Nataraj**, Vibrational (FT-IR and FT-Raman) spectra, NBO, HOMO–LUMO, Molecular electrostatic potential surface and computational analysis of 4-(trifluoromethyl)benzylbromide, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** **116 (2013) 84–95**.

17. T.Karthick, V.Balachandran, S.Perumal, **A. Nataraj**, Vibrational (FT-IR and FT-Raman) spectra and quantum chemical studies on the molecular orbital calculations, chemical reactivity and thermodynamic parameters of 2-chloro-5-(trifluoromethyl) aniline, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, **107 (2013) 72-81**.

18. T.Karthick, V.Balachandran, S.Perumal, **A. Nataraj**, Comparative theoretical studies on natural atomic orbitals, natural bond orbitals and simulated UV-visible spectra of N-(methyl)phthalimide and N-(2-bromoethyl)phthalimide, **Indian Journal of Pure & Applied Physics**, **51 (2013) 178-184**.

19. **A. Nataraj**, V.Balachandran, T.Karthick, Molecular structure, vibrational spectra, first hyperpolarizability and HOMO, LUMO analysis of p-acetylenebenzotrile using quantum chemical calculations, **Journal of Molecular Structure**, **1038 (2013) 134-144**.

20. V.Balachandran, **A. Nataraj**, T.Karthick, Molecular structure, spectroscopic (FT-IR, FT-Raman) studies and first-order molecular hyperpolarizability, NBO analysis of 2-hydroxy-p-toluic acid, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, **104 (2013) 114-129.**
21. **A. Nataraj**, V.Balachandran, T.Karthick, Molecular orbital studies (Hardness, Chemical potential, Electrophilicity, and first electron excitation), vibrational investigation and theoretical NBO analysis of 2-hydroxy-5-bromobenzaldehyde by density functional method, **Journal of Molecular Structure**, **1031(2013) 221-233.**
22. **A. Nataraj**, V.Balachandran, T.Karthick, M. Karabacak, A. Atac, FT-Raman, FT-IR, UV spectra and DFT and ab initio calculations on monomeric and dimeric structures of 3, 5-pyridinedicarboxylic acid, **Journal of Molecular Structure**, **1027 (2012) 1-14.**
23. **A. Nataraj**, V.Balachandran, T.Karthick, FTIR and Raman spectra, DFT and SQMFF calculations for geometrical interpretation and vibrational analysis of 3-nitro-p-toluic acid” **Journal of Molecular Structure**, **1022 (2012) 94-108.**
24. V.Balachandran, T.Karthick, S.Perumal, **A. Nataraj**, Vibrational spectroscopic studies, molecular orbital calculations and chemical reactivity of 6-nitro-m-toluic acid **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, **92 (2012) 137-147.**
25. **A. Nataraj**, V.Balachandran, T.Karthick, Density functional study on the structural conformations, intramolecular charge transfer and vibrational spectra of 4-hydroxy-3-methoxy-5-nitrobenzaldehyde, **Journal of Molecular Structure**, **1006 (2011) 104-112.**
26. T.Karthick, V.Balachandran, S.Perumal, **A. Nataraj**, Rotational isomers, vibrational assignments, HOMO-LUMO, NLO properties and molecular electrostatic potential surface of N-(2 bromoethyl) phthalimide, **Journal of Molecular Structure**, **1005 (2011) 202-213.**
27. T.Karthick, V.Balachandran, S.Perumal, **A. Nataraj**, Spectroscopic studies, HOMO-LUMO and NBO calculations on monomer and dimer conformer of 5-nitrosalicylic acid, **Journal of Molecular Structure** **1005 (2011) 192-201.**
28. T.Karthick, V.Balachandran, S.Perumal, **A. Nataraj**, A Density functional approach to pharmaceutical intermediate n- (methyl) phthalimide to yield complete vibrational assignments and HOMO-LUMO energy gap, **Elixir Vibrational Spectroscopy**, **36 (2011) 3388-3396.**

**BOOK PUBLISHED**

T. Beena, , L. Sudha, A. Nataraj, and G. Mariappan, DFT Computational Insights into Structural, Dielectric and Spectroscopic parameters of 2-((3,4-dichlorophenyl imino)methyl)-4-Bromophenol-A Concise Experimental Approach, Chapter 8, Print ISBN: 978-81-19491-08-7, eBook ISBN: 978-81-19491-09-4, DOI: 10.9734/bpi/cteims/v2/1097G.

#### **AICTE COURSE COMPLETED**

UHV 1: Participated and successfully completed the 5-day Online FDP on the theme “Inculcating Universal Human Values in Technical Education” organized by All India Council for Technical Education (AICTE) from 12th June to 16th June 2023. F.No AICTE/FDP-SI/OnlineWorkshop/201/191388

#### **NPTEL COURSE COMPLETED**

- ❖ Course Completed: 3 Credits: NPTEL Online Certification Course “Fundamentals of Spectroscopy” with score of 53%, 12 weeks, Jan-April, 2023.
- ❖ Course Completed: 2 Credits: NPTEL Online Certification Course “Solar Photovoltaics Fundamentals, Technology and Applications” with score of 56%, 8 weeks, July-Sept, 2022.
- ❖ ELITE: 2 Credits: NPTEL Online Certification Course “Nanotechnology in Agriculture” with score of 69%, 8 weeks, Feb-March, 2022.

#### **PROFESSIONAL BODIES**

- ❖ Life Member in **Materials Research Society of India (MRSI)**, Trichy Chapter/LMB2482
- ❖ Annual Member in Indian Science Congress Association (ISCA) A6/2024
- ❖ Life Member in Indian Association for Crystal Growth (IACG) - 302/2023

#### **REVIEWER IN REPUTED JOURNALS**

Reviewer in the reputed journal of Vibrational Spectroscopy, Optics, Journal of Molecular Structure, and Spectrochimica Acta Part A

#### **REFRESHER COURSE / SEMINAR/ PROGRAMME ATTENDED**

- ❖ Participated in the Women’s day lecture series on Magnetic Oxides and Application by Dr. Rajshree B. Jotania, Professor, Department of Physics, Electronics and Space Science, University School of Sciences, Gujarat University, Navrangpura, Ahmedabad, Gujarat, India, held on 08 th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India.

- ❖ Participated in the Women's day lecture series on An Overview of Indian Nanoelectronics User's Programme - Idea to Innovation by Dr. K Nageswari, Sr. INUP Program Manager, Indian Nanoelectronics Users Program, Dept. of Electrical Engineering, IIT Bombay, Powai, Mumbai, India, held on 08 th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India.
- ❖ Participated in the National Webinar on Research Funding Opportunities by Dr. S. Praveen Kumar, Scientist "F", Department of Science and Technology (DST), Government of India, New Delhi, India, held on 07th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India.
- ❖ Participated in the International Webinar on Zn Stannate Modified Graphitic Carbon Nitride for the Photocatalytic Removal of Hexavalent Cr in H<sub>2</sub>O by Dr. Damian C. Onwudiwe, Professor, Department of Chemistry, North-West University (NWU), Mahikeng Campus, South Africa, held on 06th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India
- ❖ Participated in the Women's day lecture series on Magneto-caloric Materials : Magnetic Cooling for Green Refrigeration by Dr. Vasundhara Mutta, Principal Scientist, CSIR-Indian Institute of Chemical Technology, Uppal Road, Tarnaka, Hyderabad, Telangana State, India, held on 08th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India.
- ❖ Participated in the National Level Seminar on "High Pressure Techniques For Structural, Magnetic And Electrical Characterizations" organized by Department of Physics, Kongunadu College of Engineering and Technology (Autonomous), Trichy on 14th March 2023.
- ❖ Participated in One-week Faculty Development Program on "Polymer Composites For Engineering Applications (PCEA-2023)" (blended-mode) held from 22nd to 26th May 2023, conducted by the Department of Chemistry, B.M.S. College of Engineering, Bengaluru-560019
- ❖ International Faculty Development Programme on Advanced Functional Materials: Energy, Environment and Sustainable Development from 28th February to 09th March, 2023 organized by the Department of Physics, SRM TRP Engineering College, Tiruchirappalli, Tamilnadu, India.

- ❖ UGC Sponsored **Refresher Course** On “*Environmental Studies*” at Bharathiar University, Coimbatore-46, from 04.05.2007 to 24.05.2007 and obtained the Grade **A**.
- ❖ Seminar on “*Nano Science and Technology*” organized at Anna Science Centre-Planetarium, Tiruchy, on 14.10.2010.
- ❖ UGC Sponsored Autonomous Grant One Day State Level Seminar On “*Recent Advances In Laser Applications*” at Jamal Mohamed College (Autonomous), Tiruchy, on 01.03.2010.
- ❖ Workshop on “*Nanotechnology*” Organized by Quantum Nano Scientific Pvt Ltd at T. H. Roever College, Perambalur, on 19.01.2011.
- ❖ **NSS Orientation Course** conducted by Empanelled Training Institution, Madras School of Social Work from 04.09.2012 to 10.09.2012.
- ❖ **Workshop** on Powder X-ray diffraction data analysis, Department of Physics, SRM University, Ramapuram, Chennai-89 on 3<sup>rd</sup> and 4<sup>th</sup> July 2015.
- ❖ “**Virtual Internship Program on Spectroscopy**” Department of Analytical Chemistry, University of Madras, Guindy Campus, Chennai & Abinnovus Consulting Pvt. Ltd from 23.08.2021 to 27.08.2021.
- ❖ **International Virtual Seminar** on “Physics and Chemistry of Materials” on 6th, February 2021 organized by Department of Physics, Karpagam Academy of Higher Education, Coimbatore- 641021.
- ❖ **International Conference** on Solution Grown Crystals and Their Useful Applications (SGCA-2021) Organized by SSN Research Centre, SSN Institutions (Autonomous) Chennai-603110, Tamil Nadu, India in association with Indian Association for Crystal Growth (IACG) During 13-15 September 2021.
- ❖ **One week AICTE sponsored online STTP** on Emerging Trends in Nanomaterials for Electronic and optoelectronic Devices, organized by ECE, Swarnandhara College of Engineering and Technology, Kakinada from May 10 – 15, 2021.
- ❖ **Five day National Level FDP** on Advancing Towards Sustainable Teaching and Learning Pedagogy, DBT star department, Kongu Arts and Science College from 2.08.2021 to 6.8.2021.
- ❖ **International eWorkshop on Science and Technology of Emerging Materials (eSTEM – 21)** – Virutal Mode Organized by the Department of Science and Humanities, Chetnad College of Engineering and Technology, Puliur-CF Karur on 19th to 21st April 2021.

- ❖ **H.C. Verma online course** on The story of photoelectric effect, IIT Kanpur, July 15 to August 17, 2021.
- ❖ **Faculty Development Program on VIRTUAL LABS**, held virtually from 23-Aug-2021 thru 27-Aug-2021 as part of the “PALS-VLABS 2021-22 INITIATIVE with NITK Surathkal”.
- ❖ **Four Weeks Online Course** From the Big Bang to Dark Energy, University of Tokyo on April 25, 2020.
- ❖ **One-week Online Faculty Development Programme** on “The Use of Virtual Physics Labs - Creating Next Generation Teachers” by Department of Freshman Engineering, Geethanjali College of Engineering and Technology in association with Indian Society for Technical Education (ISTE).20-24, May 2020.
- ❖ **Five Days FDP on Evaluation on Teaching Learning Process** – Post Covid 19 organized by the Bharath Institute of Science and Technology, from 11<sup>th</sup> May 2020 to 15<sup>th</sup> May 2020.
- ❖ **Two Weeks Faculty Development Programme on "MANAGING ONLINE CLASSES and CO-CREATING MOOCS:2.0"** MHRD PMMMNMTT sponsored, Ramanujan College, New Delhi, from May 18 - June 03, 2020.
- ❖ **Online Course** on Adobe Photoshop CC advanced training course, Udemy, April30, 2020.
- ❖ **Two days National level workshop** on Advanced Materials Characterization Tools, held on 20-21<sup>st</sup> May 2020 organised by SRM Institute of Science and Technology, Kattankulathur.

#### **ACTIVITIES**

- ❖ Acted as a NSS Programme Officer from September 2011 to 31.4.2013 and Organized and Participated in the various concurrent programmes under NSS.
- ❖ Acted as a Hostel Deputy Warden at Muthu Mase College of Arts and Science College from July 2006 to April 2009.
- ❖ Guided - 10 M.Sc., Project.
- ❖ Invited for the Research day celebration as a Chief Guest given Special Lecture about Nanotechnology in Renewable Energy at Arignar Anna Government College, Musiri, Trichy-621211, Tamilnadu, India on 29th February 2016.