

## Papers Published by Staff in Journals

Name of the Staff	Title of the Paper	Name of the Journal with ISSN No/Impact factor/Citation Index	Volume ,Issue,Page,Year
Dr.S.R.Gibin	Preparation and characterization of nickel ferrite nano particles by co-precipitation method with citrate as chelating agent	Journal of Materials Science: Materials in Electronics, 0957-4522 Impact Factor:2.779	Volume 27, Issue 3, pp 2601–2607, 2015
Dr.S.R.Gibin	Preparation and characterization of nanosized cobalt ferrite particles by co-precipitation method with citrate as chelating agent.	Journal of Materials Science: Materials in Electronics, 0957-4522 Impact Factor:2.779	Volume 27, Issue 9, pp 8891–8898, 2016
Dr.S.R.Gibin	Synthesis and characterization of nickel cobalt ferrite ( $Ni_{1-x}Co_xFe_2O_4$ ) nano particles by co- precipitation method with citrate as chelating agent.	Journal of Materials Science: Materials in Electronics, 0957-4522 Impact Factor:2.779	Volume 28, Issue 2, pp 1985–1996, 2017
Dr.S.R.Gibin	Super Capacitance study on $Fe_3O_4$ nanoparticles prepared by citrate assisted co-precipitation method.	International Journal of Creative Research Thoughts ISSN: 2320-2882 Impact Factor:7.97	Volume 6, Issue 1 2018
Dr.S.R.Gibin	Preparation and Characterization of Nickel Substituted Copper Ferrite Nano Particles for Super Capacitance Applications via Citrate Assisted Co-precipitation Method.	Journal of Computational Information Systems ISSN : 1553-9105	Volume 14, Issue 4, pp 63-68. 2018
Dr.S.R.Gibin	Super Capacitance Study on $CuFe_2O_4$ Nanoparticles prepared by Means of Citrate Assisted Co-precipitation Method	Journal of Computational Information Systems ISSN : 1553-9105	Volume 14, Issue 4, pp 69-75. 2018
M.L.Lima Rose	Studies on thermal and biological properties of organic 4-	YMER	, Vol. 21, pp.691-700 (Scopus)

	hydroxybenzophenone single crystal, ,		
<b>Dr.A.Mariappan</b>	Synthesis and DFT computations on structural,electronic and vibrational spectra,RDG analysis and molecular docking of novel Anticovid -19 molecule 3,5 dimethyl pyrazolium 3,5 Dichloro salicylate.	<b>“Journal of Molecular Structure” –</b> 0022-2860 / I.F - 3.841 / 18	1246 & 131165, 2021
<b>Dr.A.Mariappan</b>	Study of the photocatalytic and antibacterial effect of Zn and Cu doped hydroxyapatite.	<b>“ Inorganic chemistry Communications” -</b> 1387 -7003 / I.F - 3.428/ <b>3</b>	136 & 109128 , 2022
<b>Dr.A.Mariappan</b>	Synthesis and characterization of Mn doped copperoxide nanoparticles	<b>AIP Conference proceedings /2464/ I.F -1.402/ 2</b>	020005& 2022
<b>Dr.A.Mariappan</b>	Structural, Optical and Antimicrobial activity of Copper and Zinc Hydroxyapatite Nanopowders using Sol-Gel Method.	<b>Machanics, Materials Science and Engineering.</b>  <b>ISSN No</b> 2412-5954 / 1.73 /23	6 & 32 – 38 , 2015
<b>Dr.A.Mariappan</b>	Antibacterial activities of HAp-TiO <sub>2</sub> Composites, Sol-	<b>Indian journal of research foundation.</b>	4 &

	gel dip Coating technique.	ISSN No. 2454- 6577/1.03/ 1	27 – 35 , 2015
<b>Dr.A.Mariappan</b>	Synthesis and optical characterization of silver doped Hydroxyapatite/TiO <sub>2</sub> nanoparticles	<b>Roots International Journal of multidisciplinary Researches</b> ISSN No. 2349- 8684 Impact factor 4.075 /3	Vol.4 ,2017
<b>Dr.Joselin Beaula T.</b>	Effect of Hydrochloric Acid (HCl) on Synthesis, Spectral and Thermal Properties of Triglycine Phosphate (TGP) Single Crystals,	<b>International Journal of Current Research and Review,</b>	9, 8, 2017
<b>Dr.Joselin Beaula T.</b>	Qualitative Chemical Analysis with Novel Structural Interpretations of Kyselina 2-Naftalensulfonova,	<b>International Journal of Emerging Technologies in Engineering Research (IJETER)</b> ISSN: 2454-6410	Volume 6, Issue 1, January (2018),
<b>Dr.Joselin Beaula T.</b>	Structural Properties of Bioactive Molecule Naphthalene 2-Sulfonic Acid,	<b>Mechanics, Materials Science &amp; Engineering</b> ISSN 2412-5954 <b>Citation Index : 1</b>	, Volume 6, Issue 1, January (2018)
<b>Dr.Joselin Beaula T.</b>	Hydrogen bonded R2 (8) graph set in inducing charge transfer mechanism in guanidinium-3,5-dinitrobenzoate: A combined experimental, theoretical and Hirshfeld surface study	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 37 Impact Factor : <b>3.841</b>	5 June 2017, Pages 649-662
<b>Dr.Joselin Beaula T.</b>	Hydrogen bonding interactions and supramolecular assemblies in 2-amino guanidinium 4-methyl benzene sulphonate crystal structure: Hirshfeld surfaces and computational calculations	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 32 Impact Factor : <b>3.841</b>	Volume 1146, 15 October 2017, Pages 723-734
<b>Dr.Joselin Beaula T.</b>	Influence of intramolecular hydrogen bonding interaction on the molecular properties of N-p-tolyl-5-oxo pyrrolidine-3-carboxylic acid: A	Chemical Physics Letters <b>ISSN: 0009-2614</b> Citation Index : 16 Impact Factor : <b>2.719</b>	691 (2018) 114–121

	theoretical and experimental study		
<b>Dr.Joselin Beaula T.</b>	Hydrogen bonding interactions in 1H-1,2,3-triazole based organic crystals: experimental and theoretical analysis	Current Applied Physics ISSN 1567-1739 Citation Index : <b>15</b> Impact Factor : <b>2.856</b>	18 (2018) 774–784
<b>Dr.Joselin Beaula T.</b>	Effect of charge transfer with spectral analysis on the antibacterial compound 4-(Dimethyl amino) pyridine: 3, 5-Dinitrobenzoic acid: Experimental and theoretical perspective	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : <b>11</b> Impact Factor : <b>3.841</b>	1171,2018, 511-526
<b>Dr.Joselin Beaula T.</b>	Supramolecular interactions in itaconic acid: 2-amino-4,6-dimethyl pyrimidine molecular adduct - Physico chemical characterization and quantum chemical calculations	<b>Journal of Physics and Chemistry of Solids</b> <b>ISSN: 0022-3697</b> Citation Index : <b>3</b> Impact Factor : 4.383	129 (2019) 284–292
<b>Dr.Joselin Beaula T.</b>	Quantum chemical calculations, structural, spectral and nonlinear optical investigations of a novel crystal N,N'-diphenylguanidinium 3,5-dichlorobenzoate	<b>Journal of Physics and Chemistry of Solids</b> <b>ISSN: 0022-3697</b> Citation Index : <b>17</b> Impact Factor : 4.383	
<b>Dr.Joselin Beaula T.</b>	Experimental and theoretical investigations of a proton transfersupramolecular adduct, aminoguanidinium p-nitrophenolate:p-nitrophenol	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : <b>1</b> Impact Factor : <b>3.841</b>	1178 (2019) 192-200
<b>Dr.Joselin Beaula T.</b>	Tuning the Computational Evaluation of Spectroscopic, ELF, LOL, NCI analysis and Molecular Docking of Novel Anti COVID-19 Molecule 4-Dimethylamino Pyridinium 3, 5-Dichlorosalicylate	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy. ISSN 1386-1425 Citation Index : <b>16</b> Impact Factor : <b>4.831</b>	259 (2021) 119907
<b>Dr.Joselin Beaula T.</b>	Insights into Weak and Covalent Interactions, Reactivity sites and	Computational and Theoretical Chemistry ISSN:	vol.1206, pp.113483,

	Pharmacokinetic Studies of 4-Dimethylaminopyridinium Salicylate Monohydrate using Quantum Chemical Computation method	2210-271X. Citation Index : 5  Impact Factor : 2.292	
<b>Dr.Joselin Beaula T.</b>	Synthesis and DFT computations on structural, electronic and vibrational spectra, RDG analysis and molecular docking of novel Anti COVID-19 molecule 3, 5-Dimethylpyrazolium 3,5-Dichloro Salicylate'	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 18 Impact Factor : 3.841	2021,vol.1246, pp. 131165
<b>Dr.Joselin Beaula T.</b>	Exploration of structural insights, spectroscopic assignments of 4-amino-6-methyl-3-thioxo-3, 4-dihydro-1, 2, 4-triazin-5 (2H) one,	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 7 Impact Factor : 3.841	vol. 1249, pp. 131559 2021
<b>Dr.Joselin Beaula T.</b>	Tuning the Computational Evaluation of Spectroscopic, ELF, LOL, NCI analysis and Molecular Docking of Novel Anti COVID-19 Molecule 4-Dimethylaminopyridinium 3, 5-Dichlorosalicylate	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, , ISSN: 1386-1425	vol.259, pp.1119907
<b>Dr.Joselin Beaula T.</b>	'Exploring the antibacterial activity of 1,2-diaminoethane hexanedionic acid by spectroscopic, electronic, ELF, LOL, RDG analysis and molecular docking studies using DFT method'	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 12 Impact Factor : 3.841	Volume 1247, 2022, 131388
<b>Dr.Joselin Beaula T.</b>	Exploration of structural insights, spectroscopic assignments of 4-amino-6-methyl-3-thioxo-3, 4-dihydro-1, 2, 4-triazin-5 (2H) one	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : 1 Impact Factor : 3.841	Volume 1249, 2022, 131559
<b>Dr.Joselin Beaula T.</b>	Quantum chemical exploration on charge transfer interactions, vibrational, topological and	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b>	Volume 1250, 2022, 131846

	molecular docking evaluation of the antimicrobial molecule 2,4,6-triallyloxy-1,3,5-triazine'	Citation Index : - Impact Factor : <b>3.841</b>	
<b>Dr.Joselin Beaula T.</b>	Probing into the Outcome of Charge Transfer Interactions and Hyperconjugative Effect on the Antibacterial Molecule 4-dimethylaminopyridine using Spectroscopic Elucidations and DFT Calculations'	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : <b>2</b> Impact Factor : <b>3.841</b>	1251, 2022,132059
<b>Dr.Joselin Beaula T.</b>	Synthesis, vibrational Depictions, IRI interpretations and docking research on coordination metal complex Diaqua aspartato zinc (II) monohydrate using DFT approach'	Journal of Molecular Liquids <b>ISSN : 0167-7322</b> Citation Index : <b>3</b> <b>Impact Factor : 6.633</b>	Vol. 351, 2022, 118687
<b>Dr.Joselin Beaula T.</b>	Computational Insights on Charge Transfer and Non-Covalent Interactions of Antibacterial Compound 4-Dimethylaminopyridinium Pyridine-2-Carboxylate Penta hydrate'	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : <b>2</b> Impact Factor : <b>3.841</b>	2022, 1256, 132525
<b>Dr.Joselin Beaula T.</b>	Effect of Charge Transfer and Non-Covalent Interactions of the synthesized NLO compound p-nitrophenol sodium-bisulfate using DFT method	<b>Polycyclic Aromatic Compounds</b> <b>ISSN: 1563-5333</b> Citation Index : - Impact Factor : <b>3.744</b>	2022, 1-23.
<b>Dr.Joselin Beaula T.</b>	Consequence of Proton Transfer and Hydrogen Bonding Interactions on the Molecular, Vibrational and Biological Properties of the Novelty Synthesized Antibacterial Compound bis-(4-Dimethylaminopyridinium) bis-(3, 5-Dinitrobenzoate) Monohydrate using DFT	<b>Journal of Molecular Structure</b> <b>ISSN: 0022-2860</b> Citation Index : - Impact Factor : <b>3.841</b>	Vol.1256, pp. 132914, 2022,

	Study		
<b>Dr.Joselin Beaula T.</b>	Impact of Protonation and Hydrogen Bonding Interactions on the Biological Properties of Antibacterial Compound 4-Dimethylaminopyridinium Salicylate Monohydrate: Correlation with Its Precursor Molecules	<b>Polycyclic Aromatic Compounds</b> <b>ISSN: 1563-5333</b> <b>Citation Index : -</b> <b>Impact Factor : 3.744</b>	2022,1-23
<b>Dr.Joselin Beaula T.</b>	Quantum Chemical Investigations on the Hydrogen-Bonded Interactions of Bioactive Molecule N2-(4-Methoxysalicylidene) Arginine Hemihydrate	<b>Polycyclic Aromatic Compounds</b> <b>ISSN: 1563-5333</b> <b>Citation Index : -</b> <b>Impact Factor : 3.744</b>	2022,1-22
<b>Dr.Joselin Beaula T.</b>	DFT Explorations on the spectral, non-covalent interactions and the invitro analysis of a synthesized anti-bacterial nanocomposite pure hydroxyapatite	Journal of Molecular Structure <b>ISSN: 0022-2860</b> <b>Citation Index : 1</b> <b>Impact Factor : 3.841</b>	vol.1264, 2022, pp.133270,
<b>Dr.Joselin Beaula T.</b>	Bioactive Small Molecule, Piperazinium Bis(4-Hydroxybenzenesulphonate) upon Spectral Investigation, Hirshfeld Surface Analysis, Molecular Docking and ADMET Prediction: A Complement DFT Calculations	<b>Polycyclic Aromatic Compounds</b> <b>ISSN: 1563-5333</b> <b>Citation Index : -</b> <b>Impact Factor : 3.744</b>	2022, 1-23
<b>Dr.Joselin Beaula T.</b>	Quantum Chemical Insights into Structural, Vibrational, Charge Transfer Excitation and NLO activity of Lithium Fumerate Dimer	Neuroquantology, ISSN: 1303-5150 <b>Citation Index : -</b> <b>Impact Factor : 0.442</b>	vol.20, 2022, no.13,pp. 3473-3490
<b>Dr PRABHA V</b>	Natural radioactivity and radiation dose measurements in agriculture soil of South India "IJRAR International Journal of Research and Analytical Reviews"	IJRAR International Journal of Research and Analytical Reviews  ISSN No 2349-5138 Impact Factor-5.75	<b>Volume 5</b> <b>Issue 4</b> <b>Page 226-235</b> <b>Year 2018</b>
<b>Dr PRABHA V</b>	Evaluation of the Gross Alpha and Beta Radioactivity	IJSRR International Journal of Scientific	<b>Volume 7</b> <b>Issue 4</b>

	Concentration in Agriculture soils of South India “ IJSRR International Journal of Scientific Research and Reviews”	Research and Reviews  Impact Factor-6.946  ISSN NO 2279-0543	<b>Page 2701-2714</b> <b>Year 2018</b>
<b>Dr PRABHA V</b>	Natural Radioactivity Levels of Virgin and Agricultural Soil Samples in South India “JASC Journal of Applied Science and Computations”	JASC Journal of Applied Science and Computations  Impact Factor-5.8  ISSN 1076-5131	<b>Volume 6</b> <b>Issue 4</b> <b>Page 3719-3728</b> <b>Year 2019</b>
<b>Dr PRABHA V</b>	Measurement of Natural Radioactivity and Hazard Indices in Agriculture Soil Using Statistical Approach “Thematics Journal of Geography”	Thematics Journal of Geography  Impact Factor-5.3  ISSN 2277-2995	<b>Volume 8</b> <b>Issue 12</b> <b>Page 91-102</b> <b>Year 2019</b>
<b>Dr PRABHA V</b>	Natural radioactivity in agriculture soil and its environmental implications in South India using Multivariate Statistical Approach, “Frontiers in Physics and Applications” (NSP-2019)	Frontiers in Physics and Applications  ISSN 978-93-84734-71-8	<b>Page 88</b> <b>Year 2019</b>
<b>Dr PRABHA V</b>	Assessment of natural Radioactivity and associated Radiological indices in soil samples of south India “Wide spectrum Research journal”	Wide spectrum Research journal  ISSN 2250-2815	<b>Page 19-27</b> <b>Year 2020</b>
<b>ANEEBA. B</b>	Polychromatic luminescence and improved antifungal performance of succinic acid in the lattice of L-Lysine monohydrochloride	Saudi Journal of Biological Sciences 1319-562X 4.052	32/ 21065-21082, Issue 16,2021
<b>ANEEBA. B</b>	Structural, optical, mechanical, electrical, and antimicrobial activities of L-Glutamine Barium Acetate (LGBA) single crystal for biological, optical and photonic applications	Journal of Materials Science: Materials in Electronics 1319-562X 2.478	28/395-399, Issue 1,2020
<b>ANEEBA. B</b>	Comprehensive studies on amino acid based organometallic L-threoninum	Journal of King Saud University-Science 1018-3647	27/2961-2967, Issue 11,2021



	cobalt (II) sulfate (LTCS) single crystal and its antibacterial and antifungal properties	3.829	
<b>ANEEDA. B</b>	Studies on physicochemical and antibacterial deeds of amino acid-based L-Threoninum sodium bromide	Saudi Journal of Biological Sciences 1319-562X 4.052	33/101443, Issue 5,2020
<b>ASHVIN SANTHIA S V</b>	Optical, dielectric and polarizability parameters of l-glutamic acid hydrochloride crystal for efficient nonlinear optical application'	Journal of Materials Science: Materials in Electronics, 1319-562X	32/16961- 16969, Issue 12,2020

### Papers/Posters Presented by Staff in Proceedings

<b>Date</b>	<b>Name of the Staff</b>	<b>Title of the Paper</b>	<b>Name of the Book/Proceedings ISBN</b>	<b>Name of the Seminar/Conference</b>	<b>State/National/International</b>	<b>Venue</b>	<b>Oral / Poster</b>
	M.L.Li ma Rose	Growth and Characterization of 2,4-dihydroxybenzophenone single crystal'		international conference in Engineering, Technology and Applied Sciences		Arunachala College of Engineering for women.	
March 26, 2022.	M.L.Li ma Rose	The studies on organic 4-hydroxybenzophenone single crystal		national conference on Advanced Materials	Department of physics, Nanjil Catholic College of Arts and science		
6&7 June 2022	M.L.Li ma Rose	The thermal property of 4-hydroxybenzophenone		National Conference on Emerging	St. Dominic's College Kanjirapally		

				Trends in Material Science			
February 20-22, 2012, 190	<b>T.Joselin Beaula</b>	Normal Coordinate Analysis and Quantum Mechanical Calculations of L-Histidine Perchlorate		<b>International Conference on Recent Trends in Advanced Materials (ICRAM-2012)</b> ,	<b>International</b>	VIT University, Vellore,	<b>Poster</b>
	<b>Dr.Joselin Beaula T.</b>	Quantum Chemical Computations and Normal Coordinate Analysis of 5-nitro-1H-indole-2,3-dione (5-nitroisatin).	978-93-82062-48-6	<b>International Conference on Molecular Spectroscopy of Advanced Materials and Biomolecules (IMSAB-2012)</b> , Bishop Moore College, Mavelikara, Kerala, Aug . 7-9, 2012, 139	<b>International</b>		<b>Poster</b>
Aug. 7-9, 2012	<b>Dr.Joselin Beaula T.</b>	Vibrational Spectroscopic Studies and DFT	978-93-82062-48-6	<b>International Conference on</b>	<b>International</b>	Bishop Moore College, Mavelikara,	<b>Poster</b>

		Calculations of Non Linear Optical Material L-Valinium Formate.		<b>Molecular Spectroscopy of Advanced Materials and Biomolecules (IMSAB-2012),</b>		Kerala, Aug. 7-9, 2012, 159	
Aug. 6-9, 2013	<b>Dr. Joselin Beaula T.</b>	Vibrational Analysis and Density Functional Calculations of 3-Aminomethyl Pyridinium Picrate		<b>International Conference on Perspectives in Vibrational Spectroscopy, (ICOPVS),</b>	<b>International</b>	Department of Physics, Bishop Moore College, Mavelikara, Kerala,	<b>Poster</b>
08-12 July 2014	<b>Dr. Joselin Beaula T.</b>	Chemical Computations and vibrational spectral studies of 2, 3-Pyrazinedicarboxylic Acid		<b>5th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS 2014)</b>	<b>International</b>	Mascot Hotel, Trivandrum, Kerala, India,	<b>Poster</b>
10-15 August 2014	<b>Dr. Joselin Beaula T.</b>	Normal Coordinate Analysis and structural		<b>XXIV International Conference</b>	<b>International</b>	The Friedrich Schiller University Jena,	<b>Poster</b>

		study of 4-Nitrophenol-Urea		Conference on Raman Spectroscopy (XXIV. ICORS Jena 2014),		Germany	
, Sept 1 & 2, 2011	<b>Dr. Joselin Beaulat.</b>	Density Functional Theoretical Computations and Vibrational Assignment of L <sup>-</sup> Histidinium Perchlorate	13:978-81-908538-8-0	<b>National Conference on Exploring the Frontiers of Vibrational Spectroscopy</b>	<b>national</b>	Women's Christian College, Nagercoil	<b>Poster</b>
January 23-24, 2012, 139	<b>Dr. Joselin Beaulat.</b>	Natural Bond Orbital Analysis of L-Histidinium Perchlorate		<b>National Seminar On Advances in Materials Science (NSAMS),</b>	<b>National</b>	Department of Physics, Manonmaniam Sundaranar University, Tirunelveli	<b>Poster</b>
March 1 & 2, 2012	<b>Dr. Joselin Beaulat.</b>	HOMO - LUMO Energies and Molecular electrostatic potential of L-Histidinium Perchlorate		<b>National Conference on Advances in Material Science (NCAMS-2012),</b>	<b>National</b>	Annamalai University, Annamalai Nager,	<b>Poster</b>
March 09 & 10, 2012,	<b>Dr. Joselin Beaulat.</b>	Density Functional Theoretical computations		<b>National Conference on Emerging</b>	<b>National</b>	Department of Chemistry, Nesamony Memorial	<b>Poster</b>

23		of 5-Nitro-1H-indole-2, 3-dione		<b>Trends in Quantum Chemistry (QUANTUM – 2012)</b>		Christian College, Marthandam,	
April, 20&21, 2012	<b>Dr.Joselin Beaula T.</b>	<b>HOMO LUMO Energies and electronic structure calculations on 2, 3-Pyrazine dicarboxylic acid ,</b>		<b>National Conference on Physics of New Materials (NCPNM-2012),</b>	<b>National</b>	N.I. University, Kumarakovil,	<b>Poster</b>
July 19 & 20, 2012	<b>Dr.Joselin Beaula T.</b>	Natural Bond Orbital Analysis and Density Functional Study on the nonlinear optical molecule L-Valinium Formate		<b>National Seminar on Recent Advancements in Materials Research (RAMR-2012),</b>	<b>, National</b>	Department of Physics & Research Centre, Scott Christian College (Autonomous), Nagercoil	<b>Poster</b>
Jan. 3-7, 2013,	<b>Dr.Joselin Beaula T.</b>	Vibrational Analysis and Density Functional Calculations of 2,3-pyrazinedicarboxylic Acid Dimer		<b>100<sup>th</sup> Indian Science Congress,</b>	<b>National</b>	University of Kolkatta, Kolkatta,	<b>Poster</b>
January , 23 – 25, 2013	<b>Dr.Joselin Beaula T.</b>	Vibrational Spectroscopic study and Density		<b>National Conference on Advanced</b>	<b>National</b>	PSN College of Engineering	<b>Poster</b>

		functional study of L-Valinium Format e		<b>Materials (NCPNM-2012),</b>		Tirunelveli	
14 <sup>th</sup> February, 2014	<b>Dr.Joseph Beaulac T.</b>	DFT and NCA calculations of 2 amino methyl pyridinium Picrate		<b>National Conference on Future Prospects in Multi Disciplinary Research</b>	<b>National</b>	Research Forum, Women's Christian College, Nagercoil	<b>Poster</b>
February 19 & 20, 2015	<b>Dr.Joseph Beaulac T.</b>	DFT and NCA analysis on antimicrobial 4-Nitrophenol-Urea dimer		<b>National Conference on Emerging Trends in Applied Physics (NCETAP-2015)</b>	<b>, National</b>	Lekshmiপুরam College of Arts and Science, Neyyoor	<b>Poster</b>
15&16, October 2015	<b>Dr.Joseph Beaulac T.</b>	Molecular Structural Analysis on Antifungal Compound 4-(Dimethyl Amino) Pyridine-3,5-Dinitrobenzoic Acid		<b>UGC Sponsored National Seminar on "New Horizons in Spectroscopy"</b>	<b>National</b>	Department Of Physics, St. John's College, Anchal, Kollam.	<b>Poster</b>
February 27th, 2016.	<b>Dr.Joseph Beaulac T.</b>	Biological studies of O-Tolyl Biguanide: DFT approach		<b>National Conference on Advanced Materials</b>	<b>National</b>	Department of Physics, Nanjil Catholic College of Arts and	<b>Poster</b>

				(NCAM - 2016),		Science, Kaliyakkavil ai,	
13 <sup>th</sup> and 14 <sup>th</sup> February 2014	<b>Dr Prabh a V</b>	Radionuclide concentration in the costal sand of Kanyakumari district, Tamil Nadu		Advances in Chemical and Nuclear Technology	National Conference	Nesamony Memorial Christian College, Marthandam	Oral
13 <sup>th</sup> March 2019	<b>Dr Prabh a V</b>	Natural Radioactivity in agriculture soil and its environmental implications in south India using multivariate statistical approach		National Seminar on Physics (NSP -19)	National Seminar	Women's Christian College, Nagercoil	Oral
24 <sup>th</sup> and 25 <sup>th</sup> January 2019	<b>Dr Dr Prabh a VPrabh a V</b>	Natural Radioactivity Levels of Virgin and Agricultural Soil Samples in South India		Frontiers in analytical and clinical techniques (INFACT-2019)	International conference	Noorul Islam Centre of Education, Kumaracoil Kanyakumari	Oral
23/01/2020	ANEE BA.B	Synthesis, Growth, Optical, Bandgap Energy, and Mechanical properties of Semi organic Non Linear Material	International conference on Recent Advances in Material Science, (ICRAMS 2020)	International conference on Recent Advances in Material Science, (ICRAMS 2020)	International	Mahatma Gandhi College, Kesavadasapuram, Thiruvananthapuram, Kerala, India.	Oral
January	ANEE	Magnetic and	National	National	National	PGP College	Oral

23, 2019,	BA. B	Structural Studies on ZnFe <sub>3</sub> O <sub>4</sub> nanoparticles by Co-precipitation method”	conference on Recent Trends in Advanced Material,	conference on Recent Trends in Advanced Material,		of Arts and Science, Namakkal, Tamil Nadu, India.	1
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### Staff as Resource Person

Date	Name of the Staff	Title of the Activity	Organiser
10/6/2022	Dr.S.R.Gibin	Delivered Motivation speech regarding current scenario of Physics	Department of Physics NMCC,Marthandam



15-17 February 2023	Dr. T. Joselin Beaula	Hands on Training on normal coordinate analysis using MOLVIB software	Department of Physics and Chemistry St. Dominic's College Kanjirapally Kerala-686512
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### Books Published by Staff

<b>Author</b>	<b>Title of the Book</b>	<b>ISBN</b>	<b>Date of Publication</b>	<b>Publishers</b>
Dr.S.R.Gibin	Ferrite based nanocomposites for supercapitance application	ISBN No. 978- 93-88761-56-7	22-08-2020	Cape Comorin publisher kanniyakumari, Tamilnadu


### Patent Published by Staff

<b>Author</b>	<b>Title of the Patent</b>	<b>FIELD</b>	<b>Date of Publication</b>	<b>Publishers</b>
Dr.S.R.Gibin	Ultrafast thermal novel thermal barrier coatings for YSZ coating.	Metallurgy	18-02-2022	Intellectual Property India
T. Joselin Beaula	Growth, Structural, Thermal, Optical and Electrical properties of Potassium Succinate succinic Acid Crystal		06/08/2021	The Patent Office Journal, No. 32/2021

### Paper Presentation by Students

Date	Name of the Student	Title of the Paper	Name of the Seminar	Venu/Organiser	International/National/Regional
January 25, 2019,	Vincy, CD	Molecular interaction analysis of N <sup>2</sup> -(4-Methoxysalicylidene) Arginine Hemihydrate DFT approach',	Proceedings of international conference on Functional materials and nanotechnology (ICFMN-2019)	Annai Velankanni College, Tholayavattam-629157,	International
February 22, 2019.	Vincy, CD	Vibrational spectral and DFT studies of N <sub>2</sub> -(4-Methoxysalicylidene) Arginine Hemihydrate,	International conference on Recent Perspectives in Research	Women's Christian College, Nagercoil,	International
March 16, 2019	Vincy, CD	Molecular Charge Transfer Excitation Analysis of N <sub>2</sub> -(4-Methoxysalicylidene) Arginine Hemihydrate a DFT Approach,	National Conference on Advanced Materials (NCAM-2019),	Nanjil Catholic College of Arts and Science, Kaliyakkavilai,	National
September 20 & 21, 2019.	Vincy, CD	Electronic Spectral Analysis of N <sub>2</sub> -(4-Methoxysalicylidene) Arginine Hemihydrate	All India Conference of KAAS,	Malankara Catholic College, Mariagiri	
April 9, 2021,	C.L.Shiny,	'Molecular docking, Quantum Chemical Computational and	National seminar on Anticancer drugs from	Chikkanna Government Arts College, Tirupur,	

		Drug likeness Studies on Paranitrophenol Sodiumbisulfate (PNSS): Antimicrobial Agent',	Nano Composite Materials (NSADNC 2021),		
2021	<b>C.L.Shiny</b>	Growth and Vibrational Spectral Investigations of Paranitrophenol Sodiumbisulphate,	Proceedings of the international virtual conference on advances in chemistry and materials,	Saveetha engineering college, Chennai	
March 26,2022	<b>C.L.Shiny</b>	Evaluation on Molecular Structure, MEP, HOMO-LUMO analysis of Synthesized Compound p-nitrophenol sodium-bisulfate,	Fourth National Conference onAdvanced Materials (NCAM-2022),	Nanjil Catholic College, Kaliyakavilai	National
May 12,2022	<b>C.L.Shiny</b>	Quantum Computational Evaluation on Molecular Structure and Wavefunction Analyses on p-nitrophenol sodium-bisulfate,	National Conference on Recent Trends in Physics (NCRTP-2022),	Noorul Islam Center for Higher Education, Kumaracoil	National
April 21-22,2022	<b>C.L.Shiny</b>	Exploration of Structural Characterization and Charge Transfer Interactions of Lithium Fumarate,	Two Days International Conference on Contemporary Research on Multiprobes Smart Materials (CRMSM),	Vivekanandha College of Arts and Sciences for Women (Autonomous)	International
March 26, 2022	Dexlin, XDD	Molecular Optimization and NCI analysis of anti-	Fourth National conference on advanced	Nanjil Catholic College of	National

		viral molecule Diaqua aspartato zinc (II) monohydrate	materials at	Arts & Science, Kaliyakkavila i,	
2021	Tarika, JDD	Exploring the bioactivity of 4- dimethyl aminopyridinium salicylate monohydrate by molecular docking and ADMET analysis'	Proceedings of the international virtual conference on advances in chemistry and materials,	Saveetha engineering college, Chennai,	International
2021,	Tarika, JDD	Charge Transfer interactions and Topological analysis of 4- dimethylaminopyridi nium salicylate monohydrate: A DFT approach'	Proceedings of the international virtual conference on smart materials chemistry (CHEMSMAT- 21),	PG and Research department of chemistry, St. Joseph's college, Trichy, July 29-31	
April 9, 2021	Tarika, JDD,	Quantum Chemical Insights on the structure, Molecular Docking and Drug likeness of Antibacterial compound 1,2 Diaminoethane Hexanedionic Acid'	National seminar on Anticancer drugs from Nano Composite Materials (NSADNC 2021), Chikkanna ,	Government Arts College, Tirupur,	
Februar y 24-28, 2020,	Tarika, JDD	Insights on the structural analysis and aromaticity of 3,5-Dichlorosalicylic Acid 4- Dimethylamino Pyridine based on computational studies	International conference on Perspectives in Vibrational Spectroscopy	JNCASR, Bengaluru	
Februar y 24-28, 2020,	Tarika, JDD	Insights on the structural analysis and aromaticity of 3,5-Dichlorosalicylic	International conference on Perspectives in Vibrational Spectroscopy,	JNCASR, Bengaluru,	International

		Acid 4-Dimethylamino Pyridine based on computational studies			
February 22, 2020.	Tarika, JDD	A Comprehensive study in the quantum chemical computation of 3, 5, Dichlorosalicylic Acid 4-Dimethyl Amino Pyridine”,	International conference on Innovative Trends in Technology & Educational Research,	Sree Ayyappa College for Women, Chunkankada i, Nagercoil,	International
February 3- 4, 2020	Tarika, JDD	Optimization and Charge distribution of 3,5-Dichlorosalicylic Acid 4-Dimethylamino pyridine based on computational studies	International conference on Chemical Science and Technology,	Srinivasan College of Arts and Science, Perambalur,	International
	Tarika, JDD	Optimization and Charge analysis of L-Phenylalaninium Methane Sulfonate using DFT method”,	All India Conference of KAAS,	Malankara Catholic College, Mariagiri, September 20 & 21, 2019,	
February 22, 2020.	Tarika, JDD,	A Comprehensive study in the quantum chemical computation of 3, 5, Dichlorosalicylic Acid 4-Dimethyl	International conference on Innovative Trends in Technology & Educational Research,	Sree Ayyappa College for Women, Chunkankada i, Nagercoil,	International

		Amino Pyridine			
February 3- 4, 2020	Tarika, JDD,	Optimization and Charge distribution of 3,5-Dichlorosalicylic Acid 4-Dimethylamino pyridine based on computational studies	International conference on Chemical Science and Technology, at,	Srinivasan College of Arts and Science, Perambalur	International
2019	Tarika, JDD	“Optimization and Charge analysis of L-Phenylalaninium Methane Sulfonate using DFT method”,	All India Conference of KAAS,	Malankara Catholic College, Mariagiri, September 20 & 21	
June 6 & 7, 2022	Tarika JDD	Probing into the Antibacterial Evaluation and Pharmacokinetic properties of 4-Dimethylaminopyridine using DFT approach	National Conference on Emerging Trends in Material Science (NCETMS 2022),		
May 12, 2022	Tarika	Investigations on the Reactivity Site Analysis, Charge Transfer And Non-Covalent Interaction Of 4-Dimethylaminopyridinium Pyridine-2-Carboxylate Pentahydrate	National Conference on Recent Trends in Physics 2022, (NCRTP-2022)	Noorul Islam Center for Higher Education, Kumaracoil	National
	Tarika	Exploring the Covalent, Non-Covalent interactions and Pharmacokinetics properties of the Antibacterial	Fourth National Conference on Advanced Materials (NCAM-2022)	Nanjil Catholic College, Kaliyakavilai	National

		compound 4-Dimethylaminopyridinium Salicylate Monohydrate			
9-10 <sup>th</sup> December	Reshma J S	Biological Potential and Spectroscopic Elucidation of Edible Wild Cycas Circinalis Seed Extracts – A DFT approach on 3,5 Dimethylpyrazole Benzilic Acid	International Seminar on Luminescence Materials [ ISLM-2022]	House boat, Alleppey, Kerala, India	International
March 26, 2022	R.S. Bemina,	Exploring the Covalent, Non-Covalent interactions and Pharmacokinetics properties of the Antibacterial compound 4-Dimethylaminopyridinium Salicylate Monohydrate	Fourth National Conference on Advanced Materials (NCAM-2022)	Department of Physics, Nanjil Catholic College of Arts and Science- Kaliyakkavilai	
9-10 December 2022	BEMIN A R. S	Structural Analysis of Metal Complex Ni(II)-3-hydroxy-2-(3-nitrophenyl)-4H-chromen-4-one	International Seminar on Luminescence Materials [ ISLM-2022]	House boat, Alleppey, Kerala, India	International
11-12 January 2023	BEMIN A R. S.,	Charge Analysis of Metal Complex Ni(II)-3-hydroxy-2-(3-nitrophenyl)-4H-chromen-4-one by DFT Studies	International Conference on Recent Advancement in Material Science and It's Applications (ICRAMSA'23)	Mannar Tirumalai Naicker Colege (Autonomous ) Pasumalai, Madurai, Tamil Nadu, India	International
28 February 2023	BEMIN A R. S.	FMO AND ESP Analysis of Metal Complex Cu (II)-3 Hydroxy -2-(3-Nitrophenyl) 4H –Chromen–4-One by DFT Studies	<b>2nd International Virtual Conference on Material Science and Nanotechnology</b>	ST. JOSEPH COLLEGE OF ARTS AND SCIENCE FOR WOMEN,	International



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### Awards Received by Faculty

Name of the Staff	Name of the Award	Title of the Paper	Name of Awarding Agency	Date and Year of Award
<b>Dr.S.R.Gibin</b>	Best researcher award	Best researcher 2020	Cape Comorin	30/12/2020
<b>Dr. Joselin Beaula T</b>	<b>Best Poster Award</b>	DFT and NCA analysis on antimicrobial 4-Nitrophenol-Urea dimer	<b>National Conference on Emerging Trends in Applied Physics (NCETAP-2015),</b> Lekshmipuram College of Arts and Science, Neyyoor	February 19 & 20, 2015
<b>Dr. Joselin Beaula T</b>	Best researcher Award		Kumari Mangrove Foundations, kandanvilai, Kanyakumai	05-09 - 2022
<b>Dr. Joselin Beaula T</b>	Best Faculty Award		Kumari Mangrove Foundations, kandanvilai, Kanyakumai	05-09 - 2022

**Seminar/ Workshop attended by Staff**

<b>Name of the staff</b>	<b>Name of the workshop /Seminar attended</b>	<b>National/International/State /University level</b>	<b>Date</b>	<b>Venue</b>
<b>Dr Prabha V</b>	Non-Power Applications of Nuclear Energy	National seminar	March 7 <sup>th</sup> &8 <sup>th</sup> 2019.	Scott Christian College, Nagercoil
<b>Dr Prabha V</b>	Nuclear Power-Clean Energy for Green Future NSNPCEGF-	National seminar	2 <sup>nd</sup> September, 2016	Pioneer Kumaraswamy College, Nagercoil

	16			
<b>Dr Prabha V</b>	Nuclear Science Programme	National Seminar	2 <sup>nd</sup> March 2017	Women's Christian College, Nagercoil