

**SRI VENKATESWARA COLLEGE OF ENGINEERING
(AUTONOMOUS), SRIPERUMBUDUR**

Department of Applied Physics

List of Publications

S.No	Name of the Faculty (all co-authors)	Title of the paper	Name of the Journal Vol. No, pages
1	G. Bharathy , Johanan Christian Prasana , V.S. Jeba Reeda , M. Prasath , A. Manikandan	Molecular structural, vibrational spectra, dual descriptor, electronic transition and biological evaluations of ethyl 4-hydroxy-3-methoxycinnamate using density functional theory	Chemical Physics Impact, Vol 8, 2024
2	R. Revathi, A. Ashok, G. Anitha,* , Anuj Kumar, M. Sukumar ,, S. Revathi,, Abdullah M. Al-Enizi, M. Sundararajan,* , Bidhan Pandit, Manish Gupta, Chandra Sekhar Dash, S. Yuvaraj, and Mohd Ubaidullah	Impact of In ³⁺ doped BiFeO ₃ nanoparticles prepared by direct combustion method: structural, elemental, optical, vibrational, morphology and magnetic studies	J Mater Sci: Mater Electron, Vol 35,PP 1-10,2024
3	R. Revathi · M. Sukumar · Anuj Kumar · Manish Gupta · P. Aji Udhaya · Satbir S. Sehgal · Bidhan Pandit · M. Sundararajan8 · A. Subramani · Chandra Sekhar Dash · N. Senthilkumar · Mohd Ubaidullah	Facile Synthesis of Ni ²⁺ Doped MgFe ₂ O ₄ Spinel Nanoparticles: Structural, Optical, Magnetic, and Dielectric Behavior	Journal of Inorganic and Organometallic Polymers and Materials Vol 34, PP 374-386, 2024
4	R. Josphineleela,†, G. Diwakarb, T. Senthilnathanc , Hanumant Sharan Singhd, K.R. Senthil Kumare, M. Anusuyaf	Experimental study on the effects of modification with nanoclay on the properties of an SMA mixture	Materials Today: Proceedings, PP 1-6, 2023

5	R. Revathia, S. Revathib, R. Jothiramalingamc,, M. Sukumar , N. Mohamed Basithe, M. Sundararajanf,, S. Yuvarajg, S. Arokiyarajh	Green synthesis of emerging ZnO and Ca-doped ZnO nanoparticles towards optical, magnetic properties and its antibacterial application	Digest Journal of Nanomaterials and Biostructures, Vol 18, NO 34 PP 1587-1597, 2023
6	G. Anithaa*, R. Jothiramalingamb , M. Sukumar , A. Ronibossd, S. Yuvaraje, G. Ramkumara, M. Sundararajanf, S. Arokiyarajg	Influence of Sr ²⁺ substitution on structural, optical and catalytic properties of CoAl ₂ O ₄ nanoparticles	Digest Journal of Nanomaterials and Biostructures, Vol 18, NO 3 PP 915-925, 2023
7	M. Sukumar ,, Jothi Ramalingam Rajabathar , Hamad AL-Lohedan , S. Suresh ,Chandra Sekhar Dash , M. Sundararajan ,, Partha Sarathi Subudhi , Selvaraj Arokiyaraj ,Ekrem Yanmaz, S. Yuvaraj , R.S. Rimal Isaac	Synthesize and characterization of copper doped nickel ferritenanoparticles effect on magnetic properties and visible light catalysis for rhodamine dye degradation mechanism	Journal of Alloys and Compounds, Volume 953, 25 Page 1-16, 2023
8	N. Subhashini,a S. Revathi, Mohd Ubaidullah, Abdullah M. Al-Enizi, S. Muthulakshmi, D. Thiripurasundari,a Shoyebmohamad F. Shaikh, Ayman Nafady,Meera Moydeen Abdulhameed,b Nouf B. Alanzi, Rayana Ibrahim Alkhalifah,Chandra Sekhar Dash, M.	Gd ³⁺ -substituted BiFeO ₃ perovskite nanoparticles: facile synthesis, characterization, and applications in heterogeneous catalysis,	Dalton Transactions V 52, pp 2735-2748, 2023

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9	P. Rajeswaran , A. Alfind Paul Frit , R. Rajesh, B. Vijayakumar , Pradeep Katta , N.R. Sheela , S. Muthu	Quantum computational, spectroscopic and molecular docking studies on 6-amino-3-bromo-2-methylpyridine,	Journal of the Indian Chemical Society, V 100, pp 1-9,,2023
10	C. Charanya , S. Sampathkrishnan , R. Kumuth, J. Praveena, A. Bhaskaran, A.Prabakar and N. Balamurugan	Synthesis, Quantum Computational Analysis and Molecular Docking of 3-(2-Hydroxyphenyl)-1-Phenyl Propanone: A Combined Experimental and Theoretical Analysis.	Polycyclic Aromatic Compounds, Online Journal page 1-20, 2022
11	S.Rajesh, S.Muthu, N.R.Sheela,	Investigations of 6-Fluoro-4-Oxo-3,4-Dihydro-2H-Chromene-2-Carboxylic Acid by Quantum Computational, Spectroscopic, TD-DFT with Various Solvents and Molecular Docking Studies,	Polycyclic Aromatic compounds, 2022
12	R.Rajesh, S.Muthu. & N.R.Sheela	Effect of Amino, Chloro, and Methyl Functional Groups on 4-(4-Hydroxyphenyl) Piperazine by Density Functional Theory and Molecular Docking Studies	Journal of Polycyclic Aromatic Compounds, Vol 41 2022
13	C. Charanya, S. Sampathkrishnan & N. Balamurugan	Molecular Docking and Quantum Chemical Computations of 4-Chloro-2-[(furan-2-ylmethyl)amino]-5-sulfamoylbenzoic Acid Based on Density Functional Theory,	Polycyclic Aromatic Compounds, Volume 43 issue 1 PP 826-849, 2022
14	<u>B. R. Raajaraman</u> , N. R. Sheela & <u>S. Muthu</u>	Spectroscopic, quantum computational, molecular docking and biological parameters of 4-phenylbutyrophenone: a neuroleptic agent,	Chemical Paper , Vol. 75, PP 3931-3948,2021
15	G. Bharathy , Johanan Christian Prasana , S. Muthu, Ahmad Irfan, Fazilath Basha Asif A. Saral S. Aayisha , R. Niranjana devi	Evaluation of electronic and biological interactions betweenN-[4-(Ethylsulfamoyl)phenyl]acetamide and some polar liquids (IEFPCMsolvation model) with Fukui function and molecular docking analysis,	Journal of Molecular Liquids,340, 2021

16	S.Arul, T.Senthilnathan , V.Jeevandam, Atishkumar	Pseudocapacitive Characteristics of Mg Doped ZnO Nanospheres Prepared by Coprecipitation Journal;	Archives of Metallurgy and Materals. Volume: 66 Number: 4 PP 1141-1148,2021
17	C. Charanya, S. Sampathkrishnan & N. Balamurugan	Quantum Chemical Computations, Molecular Docking, Experimental and DFT Calculation of 4-Amino-3-Phenylbutanoic Acid,	Polycyclic Aromatic Compounds, Volume 42 issue 4 page 1302-1321,2020
18	B.R.Rajaraman, N.R.Sheela , S.Muthu.	Quantum Chemical, Vibrational Spectroscopic and Molecular Docking Studies of 1- (diphenylmethyl) piperazine.	Polycyclic Aromatic Compounds, Online Journal page 1-22, 2020.
19.	C. Chranya, S. Sampathkrishnan , N. Balamurugan	Quantum Chemical Computations, Molecular Docking, Vibrational Spectroscopic Analysis, Non-Linear Optical Properties and DFT Calculation of 2-[(2,3- Dimethylphenyl) Amino]Benzoic Acid	Polycyclic Aromatic Compounds Dec 2019 Online Journal
20	C. Chranya, S. Sampathkrishnan , N. Balamurugan	Quantum Chemical Studies, Spectroscopic Analysis and Molecular Structure Investigation of 4-Chloro-2-[(Furan-2- Ylmethyl)Amino]-5-Sulfamoylbenzoic acid	Macedonian Journal of Chemistry and Chemical Engineering Vol. 38, No. 2, 2019
21	Rubarani. P.Gangadharan S.Sampath Krishnan and M. Thirumalaikumar	Quantum chemical and Corrosion Inhibition studies of (4-Chlorophenyl)-N-(4-Methylphenl) Nitroene	Spectroscopy and Spectral Analysis Vol.39, No.12, pp. 3940-3945,2019
22	BR. Raajaraman , N.R. Sheela , S. Muthu	Influence of acetyl, hydroxy and methyl functional groups on 2-phenylbutanoic acid by quantum computational, spectroscopic and ligand-protein docking studies	Journal of Molecular Structure Vol 1188 (2019) pp.99-109
23	BR Raajaramana , N.R. Sheela , S. Muthu	Spectroscopic, quantum computational and molecular docking studies on 1-phenylcyclopentane carboxylic acid	Computational Biology and Chemistry vol . 82 (2019) 44-56
24	Ramesh Babu A Dr. A. Bhaskaran Sudharashanam M Prabhu A	Performance, combustion and emission characteristics of a single-cylinder constant speed compression ignition engine using soybean methyl esters	International Journal of Ambient Energy, https://doi.org/10.1080/01430750.2018.1472659

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28	Ruba Rani P Gangadharan . S.Sampathkrishnan	Quantum Chemical Calculation on 4-[2(tert-Butylamino)-(1 hydroxyethyl)] Phenol by Density functional Theory	Spectroscopy and Spectral analysis, Vol 38, pp.3681-3637, Nov. 2018
29	Saranya CDr. S.Sampathkrishnan Balamurugan N	Natural Bond orbital, Natural population analysis of atomic charges of 4 amino- 3 phenylbutanoic acid	Spectroscopy and Spectral analysis, Vol 39, pp. 3 March. 2019
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65	S. MUTHU and S. Renuga	Vibrational spectra and normal coordinate analysis of 2-hydroxy-3-(2-methoxyphenoxy) propyl carbamate	<i>SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy Elsevier Volume 132, 11 2014, Pages 313-325</i>
66	S, MUTHU, Arunachalamprabakaran	Scaled Quantum Chemical Studies of the Molecular Structure and Vibrational Spectra of Minoxidil	Spectroscopy Letters. Taylor & Francis Group Vol.48: 63–73, 2015
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69	K. Bhavani, S. Renuga, S. MUTHU, K. Sankaranarayanan	Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, ¹³ C, ¹ H) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2-acetoxybenzoic acid by density functional methods	<i>SpectrochimicaActa Part A: Elsevier Volume 136, Part C, 5 2015, Pages 1260-1268</i>

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71	E. ElamuruguPorchelvi, S. MUTHU	<u>Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, thermodynamic analysis and normal coordinate analysis of Salicylaldehydep-methylphenylthiosemicarbazone by density functional method</u>	<i>SpectrochimicaActa Part A: Elsevier Volume 134, 5 2015, Pages 453-464</i>
72	S. Sakthivel, T. Alagesan, Abdulaziz A. Al-Saadi, S. Renuga, S. MUTHU	Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: Combined experimental and theoretical studies	<i>SpectrochimicaActa Part A: Elsevier Volume 127, 5 2014, Pages 157-167</i>
73	R. Shahidha, Abdulaziz A. Al-Saadi,S. MUTHU	Vibrational spectroscopic studies, normal co-ordinate analysis, first order hyperpolarizability, HOMO–LUMO of midodrine by using density functional methods	<i>SpectrochimicaActa Part A: Elsevier Volume 134, 5 2015, Pages 127-142</i>
74	S. MUTHU, E. ElamuruguPorchelvi, M. Karabacak, A.M. Asiri, Sushmita S. Swathi	Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehydep-chlorophenylthiosemicarbazone	<i>Journal of Molecular Structure, Elsevier Volume 1081, 5 2015, Pages 400-412</i>
75	N. Swarnalatha, S. Gunasekaran, S. MUTHU, M. Nagarajan	Molecular structure analysis and spectroscopic characterization of 9-methoxy-2H-furo[3,2-g]chromen-2-one with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations	<i>SpectrochimicaActa Part A: Elsevier Volume 137, 25 2015, Pages 721-729</i>
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77	S. Renuga , M. Karthikesan, S. MUTHU	FTIR and Raman spectra, electronic spectra and normal coordinate analysis of N,N-dimethyl-3-phenyl-3-pyridin-2-yl-propan-1-amine by DFT method	<i>SpectrochimicaActa Part A: Elsevier Volume 127, 5 2014, Pages 439-453</i>
78	S. MUTHU , E. Elamuruguporchelvi , Anitha Varghese	DFT electronic structure calculations, spectroscopic studies, and normal coordinate analysis of 2-[(5-nitro-1,3-thiazol-2-yl)carbamoyl]phenyl acetate	<i>SpectrochimicaActa Part A: Elsevier Volume 138, 5 2015, Pages 743-752</i>
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84	N.R. SHEELA , S. Muthu, S. S.Sampathkrishnan, Abdulaziz A. Al-Saadi	Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory	<i>SpectrochimicaActa Part A: Elsevier Volume 139, 15 2015, Pages 189-199</i>

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88	S.Renuga,S.Muthu	Molecular structure, normal coordinate analysis, harmonic vibrational frequencies, NBO, HOMO–LUMO analysis and detonation properties of (S)-2-(2-oxopyrrolidin-1-yl) butanamide by density functional methods	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 118 (2014) 702–715,
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90	S. Muthu , T. Rajamani , M. Karabacak , A.M. Asiri	Vibrational and UV spectra, first order hyperpolarizability, NBO and HOMO–LUMO analysis of 4-chloro-N-(2-methyl-2,3-dihydroindol-1-yl)-3-sulfamoyl-benzamide	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 122 (2014) 1–14

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