

Important Publications

S.No.	Author(s)	Title	Name of Journal	Volume	Page	Year
1	T. Murugan a, A. Suvitha b, B. Milton Boaz	Crystal growth, structural, optical, mechanical characterization and quantum chemical analysis by DFT of an organic nonlinear optical single crystal 4-Hydroxy pyridinium succinate for photonic and optoelectronic devices	Journal of Molecular Structure	1303	137536	2024
2	R. Durgadevi, A. Suvitha, Ananth Steephen & T. Arumanayagam	Computational, experimental investigations on effect of phosphoric acid to enhance the linear and nonlinear optical properties of hexamine p-nitrophenol crystal	Optical and Quantum Electronics-Q2	56	120	2024
3	Ananth Steephen a, Karuna Saini b, A. Suvitha c, P. Vivek d, T. Arumanayagam e, M. Rekha f, Bradha	Investigational, computational explorations on betanin, lycopene, cyanidin, and peonidin organic photo sensitizers for green energy harvesting	Sustainable Energy Technologies and Assessments Q1	60	103451	2023
4	Antony Lilly Grace, M. ; Suvitha, A. ; Trilaksana, Herri ; Athikesavan, Venkatraj ; Prathap, Koyada ; Judith Jayarani, A	Temperature-dependent energy storage performance of La ₂ O ₃ doped (1-x)Bi _{0.5} (Na _{0.84} K _{0.16}) _{0.5} TiO ₃ -xSrTiO ₃ multifunctional ceramics for piezoelectric sensor applications	Journal of Materials Research (JMRS) Q2	38(22)	4902-4912	2023
5	R. Sivaranjani ^a , A. Suvitha ^b , Medhansh Garg ^b , T. Arumanayagam ^a	Exploring linear and nonlinear optical behaviour of morpholine p-nitrophenol crystal: computational and	Chemical Physics Impact	7	100363	2023

6	R. Durgadevi, A. Suvitha, Ananth Steephen & T. Arumanayagam	Computational, experimental investigations on effect of phosphoric acid to enhanced the linear and nonlinear optical properties of hexamine p- nitrophenol crystal	Optical and Quantum Electronics Q2	56	120	2023
7	P. Vivek, A. Suvitha, G. Saravana Kumar, M. Rekha,	Hypothetical, investigational explorations on potential metal organic single crystal Bis (2, 6-diaminopyridin-1-ium) hexaaquacobalt (II) disulfatedihydrate	MRS Communications	13	451-459	2023
8	Suhailah Wasman Qader1 · Mehmet Ozdemir2 · Innocent Benjamin3 · Chioma M. Chima3 · A.	Toxicity, Pharmacokinetic Profile, and Compound-Protein Interaction Study of Polygonum minus Huds Extract	Applied Biochemistry and Biotechnology-Q2 Journal	23	04499	2023
9	M. A. M. El-Mansy1,2 · D. Thanmayalaxmi3 · A. Suvitha3 · Herri Trilaksana4	Crystallographic (X rays), Spectroscopic (FT IR, FT Raman, NMR), electronic (NBO, FMOs) and NLO analyses for Zidovudine (ZDV); correlated experimental and theoretical studies	Optical and Quantum Electronics- Q2	55	490	2023
10	Herri Trilaksana1 ,Thanmayalaxmi D2 & A Suvitha2	ADMET, Pharmacokinetic and Docking properties of the fungal drug 2- (2, 4-difluorophenyl)-1, 3-bis (1, 2, 4 triazol-1-yl) propan-2-ol by using Quantum computational methods	Indian Journal of Biochemistry and Bio Physics	60	58-64	2023
11	Herri Trilaksana, Thanmayalaxmi Darbhe, Athisaya Raja Suvitha, Rajesh Gangatharan,	New Quantum approach on Epilepsy drug 3'-Aminothymidin based on Pharmacokinetic, Topological and Molecular docking report-	Bio interface Research in Applied Chemistry	13(5)	432	2023

12	BRADHA MADHAVAN, Suvitha A, Anand Steephen,	Experimental and theoretical validation studies of ASnO ₃ (A = Ba, Ca, Sr) nano fibers for bioactivity applications"	International Journal of Nanotechnology.	19(6-11)	554-565	2023
13	BRADHA MADHAVAN,Ar una Suvitha A,Nagaraj, Anand Steephen,	Optimising pharmacokinetics via ADMET, bioactivity of Zr substituted samarium- doped ceria nanomaterials	International Journal of Nanotechnology.	20	512 - 522	2023
14	Mohsen Doust Mohammadi , Hewa Y. Abdullah, Karwan W. Qadir, A.Suvitha	Utilization Of Carbon Based Nanomaterial to Sense Vinyl Chloride in the Gas Phase: Theoretical Investigation	Diamond and Related Materials /Elsevier	131	109602	2023
15	Satish Kumar Palanisamy 1 , Arun Kumar Udayakumar 2 , Azher M. Abed 3 ,	Computational, Investigational Explorations on Structural, Electro-Optic Behavior of Pelargonidin Organic Colorant for TiO ₂ Based DSSCs	Symmetry-Q1	15(1)	22	2023
16	A. Suvitha; N. Y. Maharani; Hewa Y. Abdullah; Steephen Ananth; P.	Experimental and Theoretical Analysis for the Structural, FT-IR, NLO, NBO and RDG Properties of Lindane Using DFT Technique	AIP conference proceedings	2554	050001	2023
17	Suhailah Wasman Qader a,* , A. Suvitha b,	Investigating the physicochemical properties and pharmacokinetics of curcumin employing density functional theory	Chemical Physics Impact	5	100130	2022

18	Mohamed Yahya ¹ · A. Suvitha.Asmae Bouziani ³	Structural, photophysical and optoelectronic activity of triphenylamine-based push–pull chromophores:	Optical and Quantum Electronics	54	816	2022
19	A.Suvitha	Quantum Chemical Studies on Structural, Spectroscopic, Thermochemistry, Photo-physical and Bioactivity Properties of m-Cresol	Bio interface Research in Applied Chemistry	12	1006 - 1021	2022
20	A.Suvitha	On the Viability of Divergent Donor Moieties in Malononitrile-Based Donor- π -Acceptor Photosensitizers for DSSCs: A DFT/TD-DFT Study	Journal of Physical Organic Chemistry	35	4403	2022
21	A.Suvitha	Novel La _{1-x} CaxTi _{1-y} TayO _{3-δ} perovskites with enhanced conductivity for	Journal of Alloys and Compounds	915	165370	2022
22	A.Suvitha	Growth, optical, electrical properties and DFT studies on piperidinium 4-nitrophenolate NLO single crystal	Journal of Crystal Growth	582	126512	2022
23	A.Suvitha	Diamond Morphology CuO Nanomaterial's Elastic properties, ADMET, Optical, Structural Studies, Electrical Conductivity and Antibacterial Activities Analysis	Inorganic and Nano-Metal Chemistry	52	1243-1255	2022

24	A.Suvitha	Exploring the crystal, ft-ir, optical, and nlo properties of 3,4-dichloro-6-ethyl-6h-pyrano[3,2-c]quinoline-2,5-dione (DCPQ),	Letters in Applied Nano Bio Science	12	14	2022
25	A.Suvitha	Organic hexamine p-nitrophenol crystal: growth, optical, electrical, mechanical and density functional theoretical studies for nonlinear optical applications	optical materials	127	112280	2021
26	A.Suvitha	Boosted electronic, NLO and absorption characteristics for quercetin and taxifolin; comparative experimental and DFT studies	Journal of Bio interface Research in Applied Chemistry	12	8241 - 8257	2021
27	A.Suvitha	Nonlinear optical studies geometrical descriptors, chemical properties and Topology analysis on Tetraethylammonium L-tartrate dihydrate Single Crystal	Journal of Molecular Crystals and Liquid Crystals	6	104-122	2021
28	A.Suvitha	Experimental, computational analysis of Butein and Lanceoletin for natural dye-sensitized solar cells and stabilizing efficiency by IoT	Environment, Development and Sustainability	24,	8807–8822	2021
29	A.Suvitha	Exploring the electronic and optical absorption properties for homo and hetero pyrrole-graphene quantum dots	Journal of Computational Electronics	20,	2387–2402	2021

30	A.Suvitha	Molecular structure, FT Raman, IR, NLO, NBO, HOMO-LUMO analysis, physicochemical descriptors, ADME parameters, pharmacokinetic Bioactivity report on 2, 3, 5, 6 –Tetra Chloro-P- Benzoquinone	Journal of Structural Chemistry	62,	1339–1356	2021
31	A.Suvitha	Boosted electronic, optical and NLO responses of Homo P nanoclusters via conducting polymeric substituents	Computational and theoretical chemistry	1202	113343	2021
32	A.Suvitha	Exploring crystal electronic optical and NLO properties of ethyl 4-(3,4 dimethoxy Phenyl 6 methyl 2 thioxo 1,2,3,4 tetrahydro Pyrimidine 5 carboxalate (MTTHPC)	Optical and Quantum electronics	53	424	2021
33	A. Suvitha	The adsorption of 1-Chloro-1,2,2,2-tetrafluoroethane onto the pristine, Al-, and Ga-doped boron nitride nanosheet	Iranian Journal of Science and Technology	45	1287–1300	2021
34	A Suvitha	Nonlinear Optical Crystalline Nature Bis (2, 6-Diaminopyridine) Hydrogen Phthalate Nitrate Monohydrate (APPN) : Development and its Phase	Results in Optics	3	100075	2021
35	A.Suvitha	Quantitative experimental and theoretical research using the DFT technique on the structural, UV, electronic, and FMO properties of Gammaxene	Bio interface Research in Applied Chemistry	11, 6,	14240 - 14250	2021

36	Seshan, G., Kanagasabai, S., Ananthasri, S., Kannappan, B., Suvitha, A., Jaimohan, S.M., Kanagaraj, S., Kothandan, G	Insights of structure-based pharmacophore studies and inhibitor design against Gal3 receptor through molecular dynamics simulations,	Taylor & Francis / Journal of Biomolecular Structure and Dynamics	39	6987- 6999	2021
37	A.Suvitha	Spectral investigations, NLO, NBO, HOMO-LUMO, MEP, ADME parameters of 2- methyl benzoquinone Using quantum computations and CADD technique	AIP Conference Proceedings	2162	020037	2019
38	Sudhir M. Hiremath, A. Suvitha, Ninganagouda R. Patil, Chidanandayya S. Hiremath, Seema S. Khemalapure, Subrat K.Patianayak, Veerabhadrayya S. Negalurmath, Kotresh Obelannavar, Sanja J. Armaković, Stevan,	ArmakovićSynthesis of 5- (5-methyl-benzofuran-3- ylmethyl)-3H-[1, 3, 4] oxadiazole-2-thione and investigation of its spectroscopic, reactivity, optoelectronic and drug likeness properties by combined computational and experimental approach	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	205	95–110	2018

39	Sudhir M. Hiremath, A. Suvitha, Ningangouda R. Patil, Chidanandayya S. Hiremath, Seema S. Khemalapure, Subrat K. Patanayake, Veerabhadrayya S. Negalurmath, Kotresh Obelannavar	Molecular structure, vibrational spectra, NMR, UV, NBO, NLO, HOMO-LUMO and molecular docking of 2-(4, 6-dimethyl-1-benzofuran-3-yl) acetic acid (2DBAA): Experimental and theoretical approach	Journal of Molecular Structure	1171	362-374	2018
40	A.Suvitha, S. Periandy, M. Govindarajan and P.Gayathri	FT-IR, FT-Raman spectra and HF- DFT methods and NBO, HOMO-LUMO and electronic transition studies on 2, 2,	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	138	900-912	2015
41	A.Suvitha, S. Periandy, and P.Gayathri	NBO, HOMO-LUMO, UV, NLO, NMR and vibrational analysis of veratrole using FT-IR, FT-Raman, FT-NMR spectra and HF-DFT	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	138	357-369	2015
42	A. Suvitha, S. Periandy, S. Boomadevi, M. Govindarajan	Vibrational frequency analysis, FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMO-LUMO and electronic structure	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	117	216-224	2014
43	A.Suvitha, S. Periandy, M. Govindarajan and S.Ramanlinga	Vibrational frequency analysis, HF and DFT(B3LYP and B3PW91) studies, HOMO-LUMO and electronic structure	Asian Journal of physics	23,6	1069-1078	2014

44	A.Suvitha, S. Periandy, and M. Govindarajan	Vibrational spectroscopic studies, HOMO–LUMO, NBO, UV and NMR analysis of 4-acetylpyridine	Asian Journal of physics	23,6	1053-1062	2014
45	M.Govindarajan, a, M. Karabacak, A. Suvitha, S.	FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMO–LUMO and electronic	Spectrochimica Acta Part A: Molecular and Biomolecular	89	137-148	2012
46	Umadevi M, Suvitha A, Latha K, Rajkumar BJ, Ramakrishnan .v	Spectral investigations of preferential solvation and solute-solvent interactions of 1,4-dimethylamino	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	67	(3-4):910-915	2007