Name of the faculty : **Prin. Dr. B.S. Jagdale**

Designation : **Principal**

Department : **Chemistry**

Name of the College : **Mahatma Gandhi Vidyamandir's Loknete Vyankatrao Hiray Arts, Science and Commerce College, Panchavati, Nashik-422003**

Details of Research Publications

Sr. No.	Title of the paper	Name of Journal	Year of publication	ISSN number	Online Link/Details
1.	One Pot Synthesis, Spectroscopic Characteriztion, and Computational Studies of Benzo[d][1,3]dioxol-5-yl(3-(4-isopropylphenyl)oxiran-2-yl)methanone and Benzo[d][1,3]dioxol-5-yl(3-(4-chlorophenyl)oxiran-2-yl)methanone	Asian Journal of Chemistry	2022	2456-8937	https://www.researchgate.net/publication/362182158_One_Pot_Synthesis_Spectroscopic_Characteriztion_and_Computational_Studies_of_Benzod13dioxol-5-yl3-4-isopropylphenyloxiran-2-ylmethanone_and_Benzod13dioxol-5-yl3-4-chlorophenyloxiran-2-ylmethanone
2.	Green Approach for the Synthesis of Chalcone: Review of Methods	Asian Journal of Chemistry	2022	2456-8937	https://www.researchgate.net/publication/362182163_Green_Approach_for_the_Synthesis_of_Chalcone_Review_of_Methods?_sg%5B0%5D=1xLINkgu0wKap_rikDWsJklqlsUvbO3OGYtVU7cuW1hVIXeXbkAIPie5ExvRRYwNYuSjnbMpbD90wmmyoIhEVKPXlccqplnCkUJ27VWU.ZQXZodoOQoDscsIktkiQY6tVVoyed20T-IBHHSI0HJoHdqpFqJwMjl0pKGSQf2Hs3nvvYZ6fs0cbPeYDl4Lp5A

3.	Combined Experimental and Computational Exploration of 4-(4-Bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one	Asian Journal of Chemistry	2022	2456-8937	https://www.researchgate.net/publication/362182088_Combined_Experimental_and_Computational_Exploration_of_4-4-Bromophenyl-6-34-dimethoxyphenyl-56-dihydropyrimidin-21H-one
4.	Exploration of photocatalytic performance of TiO2, Ni-doped TiO2, and Fe-doped TiO2 for degradation of eosine blue dye: comparative study	Results in Chemistry	2022	2211-7156	https://www.scopus.com/sourceid/21101024415
5.	PEG-mediated synthesis, antibacterial, antifungal and antioxidant studies of some new 1,3,5-trisubstituted 2-pyrazolines	Molecular Diversity	2022	1381-1991	https://www.scopus.com/sourceid/29053
6.	Combined Experimental and Computational Exploration of 4-(4-Bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one	Asian Journal of Chemistry	2022	2456-8937	
7.	Synthesis, molecular structure, electronic, spectroscopic, NLO and antimicrobial study of N-benzyl-2-(5-aryl-1, 3, 4-oxadiazol-2-yl) aniline derivatives	Journal of Molecular Structure	2022	0022-2860	https://www.scopus.com/sourceid/24642
8.	Photocatalytic Degradation of Methylene Blue, Rhodamine B, Methyl orange and Eriochrome Black T Dyes by Modified ZnO Nanocatalysts: A Concise Review	Inorganic Chemistry Communications	2022	1387-7003	https://www.scopus.com/sourceid/25267
9.	Nano 5% Fe–ZnO: A highly efficient and recyclable heterogeneous solid nano catalyst for the Biginelli reaction	Journal of the Indian Chemical Society	2022	0019-4522	https://www.scopus.com/sourceid/24097
10.	Fe3+ modified zinc oxide nanomaterial as an efficient, multifaceted material for photocatalytic degradation of MB dye and ethanol gas sensor as part of environmental rectification	Inorganic Chemistry Communications	2022	1387-7003	https://www.scopus.com/sourceid/25267
11.	Synthesis, spectral analysis, antibacterial, antifungal, antioxidant and hemolytic activity studies of some new 2, 5-disubstituted-1, 3, 4-oxadiazoles	Journal of Molecular Structure	2022	0022-2860	https://www.scopus.com/sourceid/24642

12.	Computational Study on Molecular Structure, UV-Visible and Vibrational Spectra and Frontier Molecular Orbital Analysis of (E)-7-((2-Chloroquinolin-3-yl) methylene)-1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one	Research Journal of Pharmacy and Technology	2022	0974-3618	https://www.scopus.com/sourceid/21100197160
13.	Synthesis and characterization of ZnO/CuO nanocomposites as an effective photocatalyst and gas sensor for environmental remediation	Journal of Inorganic and Organometallic Polymers and Materials	2022	1574-1443	https://www.scopus.com/sourceid/4700152855
14.	Photocatalytic Applications of Doped Fe 3 O 4 Nanoparticles for Degradation of Methyl Orange and Methylene Blue Dyes: A Review	Asian Journal of Organic & Medicinal Chemistry	2022	2456-8937	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
15.	Antimicrobial and computational investigation of two 2,3-dihydro-1H-inden-1-one derived fluorinated chalcone motifs	Vietnam Journal of Chemistry	2021	2572-8288	https://www.scopus.com/sourceid/21101043786
16.	Spectroscopic (FTIR and UV), quantum Chemical, antifungal and antioxidant investigations of (E)-7-(4-(trifluoromethyl) benzylidene)-1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one: A combined experimental and theoretical study	Vietnam Journal of Chemistry	2021	2572-8288	https://www.scopus.com/sourceid/21101043786
17.	Synthesis, Computational, Antibacterial and Antifungal Investigation of Two TriFluorinated Chalcones of 1-(2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)eth	Polycyclic Aromatic Compounds	2021	1040-6638	https://www.scopus.com/sourceid/26442
18.	Transition metals Fe3+, Ni2+ modified titanium dioxide (TiO2) film sensors fabricated by CPT method to sense some toxic environmental pollutant gases	Journal of the Indian Chemical Society	2021	0019-4522	https://www.scopus.com/sourceid/24097
19.	Microwave prompted solvent-free synthesis of new series of heterocyclic tagged 7- arylidene indanone hybrids and their computational, antifungal, antioxidant, and cytotoxicity study	Bioorganic Chemistry	2021	0045-2068	https://www.scopus.com/sourceid/25789

20.	Superfast synthesis, antibacterial and antifungal studies of halo-aryl and heterocyclic tagged 2, 3-dihydro-1H-inden-1-one candidates	Monatshefte für Chemie-Chemical Monthly	2021	0026-9247	https://www.scopus.com/sourceid/24803
21.	Structural, Spectroscopic (UV-Vis and IR), Electronic and Chemical Reactivity Studies of (3, 5-Diphenyl-4, 5-dihydro-1H-pyrazol-1-yl)(phenyl) methanone	Physical Chemistry Research	2021	2322-5521	https://www.scopus.com/sourceid/21100820130
22.	Synthesis, Molecular Structure, HOMO-LUMO, Chemical, Spectroscopic (UV-Vis and IR), Thermochemical Study of Ethyl 6-amino-5-cyano-2-methyl-4-(4-nitrophenyl)-4H-pyran-3-carboxylate: A DFT Exploration	Material Science Research India	2021	0973-3469	Only peer reviewed journal
23.	Synthesis, antibacterial and computational studies of Halo Chalcone hybrids from 1- (2, 3-Dihydrobenzo [b][1, 4] dioxin-6-yl) ethan-1-one	Journal of the Indian Chemical Society	2021	0019-4522	https://www.scopus.com/sourceid/24097
24.	DFT computational insights into structural, electronic and spectroscopic parameters of 2-(2-Hydrazineyl) thiazole derivatives: a concise theoretical and experimental approach	Journal of Sulfur Chemistry	2021	1741-5993	https://www.scopus.com/sourceid/24655
25.	Computational Chemistry: Sulfamic Acid Catalyzed PEG-400 Mediated Synthesis, Molecular Structure, HOMO–LUMO, UV-visible, Vibrational, and Reactivity Descriptors Analysis of 2-(Furan-2-yl)-1H-benzo[d]imidazole	Orbital: The Electronic Journal of Chemistry	2021	1984-6428	https://www.scopus.com/sourceid/21100820675
26.	PEG-400 mediated synthesis, computational, antibacterial and antifungal studies of fluorinated pyrazolines	Current Research in Green and Sustainable Chemistry	2021	2666-0865	https://www.scopus.com/sourceid/21101043776
27.	Design, fabrication, antitubercular, antibacterial, antifungal and antioxidant study of silver doped ZnO and CuO nano candidates: A comparative pharmacological study	Current Research in Green and Sustainable Chemistry	2021	2666-0865	https://www.scopus.com/sourceid/21101043776

28.	Molecular Structure, FT-IR Spectra, MEP and HOMO-LUMO Investigation of 2-(4- Fluorophenyl)-5-phenyl-1, 3, 4-oxadiazole Using DFT Theory Calculations	Advanced Journal of Chemistry-Section A	2021	2645-7768	Only peer reviewed journal
29.	Experimental and theoretical exploration on single crystal, structural, and quantum chemical parameters of (E)-7-(arylidene)-1, 2, 6, 7-tetrahydro-8 H-indeno [5, 4-b] furan-8-one derivatives: A comparative study	Journal of the Chinese Chemical Society	2021	0009-4536	https://www.scopus.com/sourceid/23449
30.	Solvent-free grindstone synthesis of four new (E)-7-(arylidene)-indanones and their structural, spectroscopic and quantum chemical study: a comprehensive theoretical and experimental exploration	Molecular Simulation	2020	0892-7022	https://www.scopus.com/sourceid/24801
31.	Molecular structure, frontier molecular orbital and spectroscopic examination on dihydropyrimidinones: a comparative computational approach	Journal of Advanced Scientific Research	2020	0976-9595	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
32.	Designing of screen-printed stannous oxide (SnO2) thick film sensors modified by cobalt and nitrogen elements for sensing some toxic gases and volatile organic compounds	Current Research in Green and Sustainable Chemistry	2020	2666-0865	https://www.scopus.com/sourceid/21101043776
33.	DFT Exploration on Molecular Characteristics of 6-Methyl-2-oxo-4-phenyl-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate	Journal of Advanced Chemical Sciences	2020	2394-5311	Only peer reviewed journal
34.	Experimental and Computational Investigations on the Molecular Structure, Vibrational Spectra, Electronic Properties, FMO and MEP Analyses of 4, 6-Bis (4-Fluorophenyl)-5, 6-dihydropyrimidin-2 (1H)-one: A DFT Insight	Physical Chemistry Research	2020	2322-5521	https://www.scopus.com/sourceid/21100820130
35.	Synthesis and DFT based quantum chemical studies of 2-(3-bromophenyl)-4-(4-bromophenyl)-2, 3-dihydro-1H-1, 5-benzodiazepine	Journal of Advanced Scientific Research	2020	0976-9595	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList

36.	Efficient synthesis, antibacterial, antifungal, antioxidant and cytotoxicity study of 2-(2- hydrazineyl) thiazole derivatives	ChemistrySelect	2020	2365-6549	https://www.scopus.com/sourceid/21100850505
37.	Aqua-mediated rapid and benign synthesis of 1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one-appended novel 2-arylidene indanones of pharmacological interest at ambient temperature	Journal of the Chinese Chemical Society	2020	0009-4536	https://www.scopus.com/sourceid/23449
38.	Transition metals Ni2+, Fe3+ incorporated modified Zno thick film sensors to monitor the environmental and industrial pollutant gases	ORIENTAL JOURNAL OF CHEMISTRY	2020	0970-020X	https://mjl.clarivate.com:/search-results?issn=0970-020X&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal
39.	Molecular structure, electronic, chemical and spectroscopic (UV-visible and IR) studies of 5-(4-chlorophenyl)-3-(3, 4-dimethoxyphenyl)-1-phenyl-4, 5-dihydro-1H-pyrazole: combined DFT and experimental exploration	Material Science Research India	2020	0973-3469	https://www.materialsciencejournal.org/specialissue2020/molecular-structure-electronic-chemical-and-spectroscopic-uv-visible-and-ir-studies-of-5-4-chlorophenyl-3-34-dimethoxyphenyl-1-phenyl-45-dihydro-1h-pyrazole-combined-dft-and-experimental-ex/
40.	Molecular structure, frontier molecular orbitals, MESP and UV–visible spectroscopy studies of Ethyl 4-(3, 4-dimethoxyphenyl)-6-methyl-2-oxo-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate: A theoretical and experimental appraisal	Material Science Research India	2020	0973-3469	https://www.materialsciencejournal.org/specialissue2020/molecular-structure-frontier-molecular-orbitals-mesp-and-uv-visible-spectroscopy-studies-of-ethyl-4-34-dimethoxyphenyl-6-methyl-2-oxo-1234-tetrahydropyrimidine-5-carboxylate-a-theoret/
41.	Efficient synthesis, spectroscopic and quantum chemical study of 2, 3- dihydrobenzofuran labelled two novel arylidene indanones: A comparative theoretical exploration	Material Science Research India	2020	0973-3469	https://www.materialsciencejournal.org/vol17no2/efficient-synthesis-spectroscopic-and-quantum-chemical-study-of-23-dihydrobenzofuran-

					labelled-two-novel-arylidene-indanones-a-comparative-theoretical-exploration/
42.	Synthesis, Spectroscopic Characterization, Quantum Chemical Study and Antimicrobial Study of (2E)-3-(2, 6-Dichlorophenyl)-1-(4-Fluoro)-Prop-2-En-1-One	Material Science Research India	2020	0973-3469	https://www.materialsciencejournal.org/vol17no3/synthesis-spectroscopic-characterization-quantum-chemical-study-and-antimicrobial-study-of-2e-3-2-6-dichlorophenyl-1-4-fluoro-prop-2-en-1-one/
43.	Experimental and Theoretical Studies on the Molecular Structure, FT-IR, NMR, HOMO, LUMO, MESP, and Reactivity Descriptors of (E)-1-(2, 3-Dihydrobenzo [b][1, 4] dioxin-6-yl)-3-(3, 4, 5-trimethoxyphenyl) prop-2-en-1-one	Material Science Research India	2020	0973-3469	https://www.materialsciencejournal.org/specialissue2020/experimental-and-theoretical-studies-on-the-molecular-structure-ft-ir-nmr-homo-lumo-mesp-and-reactivity-descriptors-of-e-1-23-dihydrobenzob14dioxin-6-yl-3-345-trimethoxyphenylprop/
44.	Investigation of Structural and Spectroscopic Parameters of Ethyl 4-(4- isopropylphenyl)-6-methyl-2-oxo-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate: a DFT Study	Chemistry & Biology Interface	2020	2249-4820	https://ugccare.unipune.ac.in/Apps1/User/WebA/AlphabetwiseList?alphabet=C
45.	Synthesis, Molecular Structure, HOMOLUMO and Spectroscopic Investigation of (E)-1-(2,4-Dichloro-5-fluorophenyl)-3- (2,6-dichlorophenyl)prop-2-en-1-one: A DFT Based Computational Exploration	Asian Journal of Organic & Medicinal Chemistry	2020	2456-8937	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
46.	Ultrasound promoted stereoselective synthesis of 2, 3-dihydrobenzofuran appended chalcones at ambient temperature	South African Journal of Chemistry	2020	0379-4350	https://www.scopus.com/sourceid/21544
47.	Structural, vibrational and chemical reactivity studies of (2-(4-chlorophenyl)-5-(4-methylphenyl)-1, 3, 4-oxadiazole	International Journal of Research and Analytical Reviews	2019	2349-5138	UGC Approved List

48.	Exploration of catalytic performance of nano-La2O3 as an efficient catalyst for dihydropyrimidinone/thione synthesis and gas sensing	Journal of Nanostructure in Chemistry	2019	2008-9244	https://mjl.clarivate.com:/search-results?issn=2008-9244&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal
49.	Synthesis, Characterization and Theoretical Study of 3-(4-bromophenyl) -5-(2,4-dichlorophenyl)-1-phenyl-4,5-dihydro-1H-pyrazole	Journal of Applicable Chemistry	2019	2278-1862	https://www.researchgate.net/publication/341312955_Synthesis_Characterization_and_Theoretical_Study_of_3-4-bromophenyl_-5-24-dichlorophenyl-1-phenyl-45-dihydro-1H-pyrazole
50.	Review on synthesis and biological activity of chalcone	International Journal of Research and Analytical Reviews	2019	2349-5138	UGC Approved List
51.	Effect of firing temperature on structural and electrical parameters of synthesized CeO2 thick films	SN Applied Sciences	2019	2523-3971	https://link.springer.com/article/10.1007/s42452-019-0246-5
52.	Zinc Oxide Nanoparticle Catalyzedbiginelli Reaction under Microwave Irradiation: An Expeditious and Green Synthesis of Dihydropyrimidinones	Researchers World: International Refereed Journal	2018	2229-4686	UGC Approved List
53.	Facile Green Synthesis of ZnO Nanoparticles, their Characterization and Gas Sensing Performance	Researchers World: International Refereed Journal	2018	2229-4686	UGC Approved List
54.	Antibacterial potential of silver nanoparticles synthesized using Madhuca longifolia flower extract as a green resource	Microbial Pathogenesis	2018	0882-4010	https://pubmed.ncbi.nlm.nih.gov/29807133/
55.	DFT Studies of 2-[(2-substitutedphenyl) carbamoyl] benzoic acids	Journal of Chemical, Biological and Physical Sciences	2017	2249-1929	https://www.researchgate.net/publication/330521391_Synthesis_Characterization_and_DFT_Studies_of_2-2-_substitutedphenyl_carbamoyl_benzoic_acids

56.	Polyethylene Glycol (PEG-400): As Green Reaction Media for Rapid Synthesis of Preparation of Isoxazolinederivatives and Its Antimicrobial Screening	International Journal of Scientific Research in Science and Technology	2017	2395-6011	https://www.researchgate.net/publication/341384837_Polyethylene_Glycol_PEG-400_As_Green_Reaction_Media_for_Rapid_Synthesis_of_Preparation_of_Isoxazolinederivatives_and_Its_Antimicrobial_Screening
57.	Molecular structure, vibrational spectra and theoretical HOMO-LUMO analysis of (E)-3, 5-dimethyl-1-phenyl-4-(p-tolyldiazenyl)-1H-pyrazole by DFT method	Der. Pharma. Chemica	2016	0975-413X	https://www.derpharmachemica.com/pharma-chemica/molecular-structure-vibrational-spectra-and-theoretical-homolumo-analysis-of-e3-5dimethyl1phenyl4ptolyldiazenyl1hpyrazol.pdf
58.	Poly (ethylene glycol)(PEG-400): A green approach towards synthesis of novel pyrazolo [3, 4-d] pyrimidin-6-amines derivatives and their antimicrobial screening	Archives of Applied Science Research	2014	0975-508X	https://www.scholarsresearchlibrary.com/articles/poly-ethylene-glycol-peg400-a-green-approach-towards-synthesis-of-novel-pyrazolo-34d-pyrimidin6amines-derivativesand-the.pdf
59.	Ultrasonic studies in mixtures of benzonitrile with some alkanols and toluene	International Journal of Pure and Applied Physics	2001	0975-1041	https://www.researchgate.net/publication/287644562_Ultrasonic_studies_in_mixtures_of_benzonitrile_with_some_alkanols_and_toluene
60.	Densities and viscosities of binary mixtures of toluene with methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol, and 2-methylpropan-2-ol at (303.15, 308.15, 313.15) K	Journal of Chemical & Engineering Data	2000	0021-9568	https://pubs.acs.org/doi/10.1021/je990317i
61.	Densities and viscosities for binary mixtures of benzonitrile with methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol, and 2-methylpropan-2-ol at (303.15, 308.15, and 313.15) K	Journal of Chemical & Engineering Data	2000	0021-9568	https://pubs.acs.org/doi/10.1021/je990237e

62.	Sonochemical studies of binary liquid mixtures of toluene with methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol, and 2-methylpropan-2-ol at 303.15, 308.15 and 313.15 K	Journal of Pure and Applied Ultrasonics	2000	0256-4637	-