**Name of the faculty** : **Dr. Vishnu Ashok Adole (M.Sc., Ph.D., CSIR-JRF, SET, GATE)**

**Designation** : **Assistant Professor**

**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 | DOI/Online link if any |
|---|---|---|---|---|---|
| 1. | DFT Calculations on Three 2,3-Dihydrobenzofuran Linked Chalcones: Structural, HOMO-LUMO and Spectroscopic (UV-Vis and IR) Interpretation | Vietnam Journal of Chemistry | 2022 | 2572-8288 | https://www.scopus.com/sourceid/21101043786 |
| 2. | Visible light prompted and modified ZnO catalyzed rapid and efficient removal of hazardous crystal violet dye from aqueous solution: A systematic experimental study | Results in Chemistry | 2022 | 2211-7156 | https://doi.org/10.1016/j.rechem.2023.100773 |
| 3. | Reactive Sensing of Gold (III) By Coumarin Tethered Fluorescent Probe Through Alkyne Activation | Journal of the Indian Chemical Society | 2022 | 0019-4522 | https://www.scopus.com/sourceid/24097 |
| 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. | 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 |

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| 7. | 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 |
| 8. | 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 |
| 9. | 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 |
| 10. | 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 |
| 11. | 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 |
| 12. | Synthesis techniques and applications of rare earth metal oxides semiconductors: A review | Chemical Physics Letters | 2022 | 0019-2614 | https://www.scopus.com/sourceid/26586 |
| 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. | PHYSICO-CHEMICAL CHARACTERISTICS OF WATER FROM WAGHDARDI DAM, MANMAD (DIST. NASHIK) AT DIFFERENT SEASONS | Pollution Research | 2022 | 0257–8050 | http://www.envirobiotechjournals.com/PR/vol41issue1/Poll%20Res-59.pdf |

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|---|---|---|---|---|---|
| 16. | Synthesis, Molecular Structure, HOMO-LUMO, Spectroscopic (UV-Vis and IR), Thermochemical Study of 5-Acetyl-4-(4-chlorophenyl)-6-methyl- 3,4-dihydropyrimidin-2(1H)-one: A DFT Study | Asian Journal of Organic & Medicinal Chemistry | 2022 | 2456-8937 | https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList |
| 17. | Interpretation of Viscometric, Thermodynamic and Acoustic Properties of Maltose in Aqueous Sodium Fluoride | Asian Journal of Organic & Medicinal Chemistry | 2022 | 2456-8937 | https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList |
| 18. | 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 |
| 19. | Fabrication, characterization and exploration of cobalt (II) ion doped, modified zinc oxide thick film sensor for gas sensing characteristics of some pernicious gases | Journal of the Indian Chemical Society | 2021 | 0019-4522 | https://www.scopus.com/sourceid/24097 |
| 20. | 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 |
| 21. | 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 |
| 22. | 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 |
| 23. | 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 |
| 24. | 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 |

| | | | | | |
|---|---|---|---|---|---|
| 25. | 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 |
| 26. | Anti-microbial evaluation, experimental and theoretical insights into molecular structure, electronic properties, and chemical reactivity of (E)-2-((1H-indol-3-yl) methylene)-2, 3-dihydro-1H-inden-1-one | Journal of Applied Organometallic Chemistry | 2021 | 2783-3623 | http://jaoc.samipubco.com/article_129274_60d3676729103cf31057580f108c3bd8.pdf |
| 27. | Synthesis and Theoretical Calculations of 2-(p-Tolyl)-2,3-Dihydro-1H-Perimidine using Density Functional Theory | Material Science Research India | 2021 | 0973-3469 | http://www.materialsciencejournal.org/vol18no1/synthesis-and-theoretical-calculations-of-2-p-tolyl-23-dihydro-1h-perimidineusing-density-functional-theory/ |
| 28. | 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 | http://www.materialsciencejournal.org/vol18no2/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/ |
| 29. | Computational Chemistry Approach for the Investigation of Structural, Electronic, Chemical and Quantum Chemical Facets of Twelve Biginelli Adducts | Journal of Applied Organometallic Chemistry | 2021 | 2783-3623 | http://jaoc.samipubco.com/article_129051_c817f8097789302f8e63e1701c9f2f7b.pdf |
| 30. | 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 |
| 31. | COMPUTATIONAL CHEMISTRY: MOLECULAR STRUCTURE, SPECTROSCOPIC (UV-VISIBLE AND IR), ELECTRONIC, CHEMICAL AND THERMOCHEMICAL ANALYSIS OF 3'-PHENYL-1, 2-DIHYDROSPIRO [INDENO [5, 4-B] FURAN-7, 2'-OXIRAN]-8 (6H)-ONE | Journal of Advanced Scientific Research | 2021 | 0976-9595 | https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList |

| | | | | | |
|---|---|---|---|---|---|
| 32. | 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 |
| 33. | Synthesis and Computational Insights on Molecular Structure, Frontier Molecular Orbital, Molecular electrostatic surface potential of (E)-3-(2,3-dihydrobenzofuran-5- yl)-1-(2-hydroxyphenyl)prop-2-en-1-one | Journal of Scientific Research | 2021 | 0447-9483 | https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList |
| 34. | 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 |
| 35. | 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 |
| 36. | 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 |
| 37. | 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 | http://www.ajchem-a.com/article_130816_f1d724ddaff1f6b30a76974ec37dd0f2.pdf |
| 38. | Synthesis, antibacterial, antifungal and DFT studies on structural, electronic and chemical reactivity of (E)-7-((1H-Indol-3-yl) methylene)-1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one | Advanced Journal of Chemistry-Section A | 2021 | 2645-7768 | http://www.ajchem-a.com/article_129397_e2edc02416d275c990e2cc923da72435.pdf |
| 39. | 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 |

| | | | | | |
|---|---|---|---|---|---|
| 40. | Density and Viscosity of LiCl, LiBr, LiI and KCl in Aqueous Methanol at 313.15 K | ORIENTAL JOURNAL OF CHEMISTRY | 2021 | 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 |
| 41. | 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 |
| 42. | 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 |
| 43. | Synthetic approaches for the synthesis of dihydropyrimidinones/thiones (biginelli adducts): a concise review | World journal of pharmaceutical research | 2020 | 2277-7105 | https://wjpr.net/abstract_file/14513 |
| 44. | Efficient synthesis, antibacterial, antifungal, antioxidant and cytotoxicity study of 2-(2- hydrazineyl) thiazole derivatives | ChemistrySelect | 2020 | 2365-6549 | https://www.scopus.com/sourceid/21100850505 |
| 45. | 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 |
| 46. | 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 |

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|---|---|---|---|---|---|
| 47. | 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/ |
| 48. | 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/ |
| 49. | 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/ |
| 50. | 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/ |
| 51. | Computational insights on molecular structure, electronic properties, and chemical reactivity of (E)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl) prop-2-en-1-one | Material Science Research India | 2020 | 0973-3469 | https://www.materialsciencejournal.org/specialissue2020/computational-insights-on-molecular-structure-electronic-properties-and-chemical-reactivity-of-e-3-4-chlorophenyl-1-2-hydroxyphenylprop-2-en-1-one/ |
| 52. | 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 |
| 53. | 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 |
| 54. | 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 |
| 55. | 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 | https://www.researchgate.net/publication/350727647_STRUCTURAL_VIBRATIONAL_AND_CHEMICAL_REACTIVITY_STUDIES_OF_2-4-_CHLOROPHENYL-5-4-METHYLPHENYL-_134-OXADIAZOLE |
| 56. | Facile Green Synthesis of ZnO Nanoparticles, their Characterization and Gas Sensing Performance | Researchers World: International Refereed Journal | 2018 | 2229-4686 | https://www.researchgate.net/publication/362283903_Facile_Green_Synthesis_of_ZnO_Nano |

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|---|---|---|---|---|---|
| | | | | | particles_their_Characterization_and_Gas_Sensing_Performance |
| 57. | AN EXPEDITIOUS AND ENVIRONMENTALLY BENIGN SYNTHESIS OF SUBSTITUTED 1,3-DIPHENYL PROP-2-EN-1-ONE | International Journal of Chemical and Physical Sciences | 2018 | 2319-6602 | https://www.researchgate.net/publication/362283862_Zinc_Oxide_Nanoparticle_Catalyzedbiginelli_Reaction_under_Microwave_Irradiation_An_Expeditious_and_Green_Synthesis_of_Dihydropyrimidinones |
| 58. | Zinc Oxide Nanoparticle Catalyzed biginelli Reaction under Microwave Irradiation: An Expeditious and Green Synthesis of Dihydropyrimidinones | Researchers World: International Refereed Journal | 2018 | 2229-4686 | https://www.researchgate.net/publication/362283862_Zinc_Oxide_Nanoparticle_Catalyzedbiginelli_Reaction_under_Microwave_Irradiation_An_Expeditious_and_Green_Synthesis_of_Dihydropyrimidinones |
| 59. | 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 |
| 60. | 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 |
| 61. | 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.researchgate.net/publication/262493870_Poly_ethylene_glycolPEG- |

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|---|---|---|---|---|---|
| | | | | | 400_A_green_approach_towards_synthesis_of_novel_pyrazolo_3_4-d_pyrimidin-6-amines_derivatives_and_their_antimicrobial_screening |