

Dr. NIVEDITA ACHARJEE

Contact: nivchem@gmail.com

Qualification: M.Sc., PhD. (University of Calcutta, Kolkata, India)

Designation: Associate Professor (West Bengal Educational Service)

Teaching Experience (UG/PG) (in years): UG: 14 years; PG: 9 years

Research Experience (in years): 17 years



Institutional Address : Department of Chemistry, Durgapur Government College, Durgapur, J. N. Avenue, District-Paschim Bardhaman, West Bengal, Pin Code-713214

Specialization/Research Interest:

The research area of Dr. Nivedita Acharjee is Computational Chemistry using conceptual Density Functional Theory (DFT) calculations for chemical systems. This research work involves studying the energetics of chemical reactions, radical spin traps, spectroscopy, photovoltaic technology and also structuring the plausible mechanism of chemical reactions. Presently, we are studying chemical reactions by the newly developed theoretical outlook "Molecular Electron Density Theory" (MEDT) proposed by Domingo in 2016.

International Research Collaborations:

- [1] Professor Luis R Domingo, Department of Organic Chemistry, University of Valencia, Spain
<http://www.luisrdomingo.com/p/colaboraciones.html>
- [2] Prof. H. A. Mohammad-Salim, Department of Chemistry, University of Zakho, Duhok 42001, Iraq
- [3] Prof. Khalid Abichhe, Applied Chemistry-Physics and Environment Team, Faculty of Sciences, Ibn Zohr University, B.P.8106 Cité Dakhla, Agadir, Morocco, Polydisciplinary Faculty of Taroudant, Ibn Zohr University, Hay El Mohammadi (Lastah), Taroudant, Morocco.
- [4] Prof. Mohammed Salah, Team of Chemoinformatics Research and Spectroscopy and Quantum Chemistry, Department of chemistry, Faculty of Science, University Chouaib Doukkali, B. P. 20, 2300, El Jadida, Morocco; LS3MN2E, Department of Chemistry, Mohammed V University, Faculty of Sciences Rabat, Morocco.
- [5] Professor Thierry Prange [Laboratoire de Cristallographie et RMN Biologiques, Université Paris Descartes, France].
- [6] Jamelah S. Al-Otaibi, Department of Chemistry, College of Science, Princess Nourah bint Abdulrahman University, Riyadh, Saudi Arabia

National Collaborations:

1. Professor Avijit Banerji [Retired Professor, University of Calcutta and Formerly Professor Ashutosh Mukherjee Fellow, National Institute for Ayurvedic Drug Development (NRIADD), West Bengal, India
2. Dr. Ani Deepthi, Department of Chemistry, University of Kerala, India
3. Dr. Madhu Ganesh, Department of Chemistry, B.M.S College of Engineering, Bull Temple Road, Bengaluru 560019, India and Department of Pharmaceutical Technology, National Institute of Pharmaceutical Education & Research, Balanagar, Hyderabad-500037, Telangana, India
4. Y. Sheena Mary and Y.Shyma Mary, Thushara, Kollam, Kerala, India

BIBLIOMETRICS

RESEARCH GATE LINK: <https://www.researchgate.net/profile/Nivedita-Acharjee>

ORCID ID: <https://orcid.org/0000-0001-8354-8693>

SCOPUS ID: <https://www.scopus.com/authid/detail.uri?authorId=34978096200>

WEB OF SCIENCE RESEARCHER ID (AAS-2991-2020): (SCI indexed publications)

<https://publons.com/researcher/3740315/nivedita-acharjee/>

VIDWAN INFLIBNET PROFILE: <https://vidwan.inflibnet.ac.in/profile/184722>

Reviewer of International Journals:

- ☞ Nature Communications (*Nature Publishing House*)
- ☞ Journal of Organic Chemistry (*American Chemical Society*)
- ☞ ACS Sustainable Resource Management (*American Chemical Society*)
- ☞ Chemistry Select (Wiley)
- ☞ New Journal of Chemistry (*Royal Society of Chemistry*)
- ☞ BMC Chemistry (*Springer-Nature*)
- ☞ Journal of Molecular Graphics and Modelling (*Elsevier*)
- ☞ International Journal of Quantum Chemistry (*Wiley*)
- ☞ Theoretical Chemistry Accounts (*Springer-Nature*)
- ☞ Chemistry-Africa (*Springer-Nature*)
- ☞ Structural Chemistry (*Springer-Nature*)
- ☞ Indian Journal of Chemistry (*NISCAIR*)
- ☞ Indian Journal of Chemistry-Section A (*NISCAIR*)
- ☞ Oriental Journal of Chemistry
- ☞ Journal of Chemical and Pharmaceutical Research

Awards & Recognitions

1. **Certificate of Recognition and Appreciation from American Chemical Society as "Peer Reviewer"**
2. **Reviewer Recognition Certificate from Elsevier**
3. **Top Downloaded Paper of 2021-2022 recognized by Wiley**
4. **Top Cited Paper of 2021-2022 recognized by Wiley**
5. **Prof. Sadhan Basu Memorial award (by University of Calcutta)** for excellence in the performance in post graduate examination, 2005.
6. **University Gold Medal** from University of Calcutta for **1st class 1st position** in M.Sc. examination in the year 2005.
7. **Umesh Chandra Memorial Cash Prize, Manoranjan Banerjee Memorial award, Pradip Kr. Ghosh Memorial Prize, Kananbala Sriti Purashkar** for first class first position in Chemistry Hons from Lady Brabourne College, Kolkata.
8. **Best poster presentation** in UGC sponsored National Level Seminar on –*Modern Trends in Chemical Sciences*|| during November 25-26, 2016 at Department of Chemistry, Prasanta Chandra Mahalanobish Mahavidyalaya.
9. **Best oral presentation** in organic Chemistry in 2nd UGC sponsored National seminar on advanced spectroscopy, theoretical chemistry, synthesis, reactivity and structure evaluation, organized by University of Burdwan, Burdwan, 20-22nd February 2009.
10. Dr. Nivedita Acharjee has contributed the first research paper of the journal "*Organics*" by MDPI in 2020 in "*Special Issue on Cycloaddition Reactions in Organic Synthesis*",1(1), 3-18. <https://doi.org/10.3390/org1010002>.
11. Dr. Nivedita Acharjee has contributed an MEDT research paper to analyse steric effects in 32CAreactions to the Special Issue "*2020 Profile Papers by Chemistry' Editorial Board Members*" of the Web of Science indexed journal "*Chemistry-Switzerland*" by MDPI in 2021 (<https://doi.org/10.3390/chemistry3010006>)
12. **NET (CSIR) 2005 with SPM shortlisting**
13. **SLET 2006 (West Bengal)**
14. **GATE 2008 (All India Rank: 25)**
15. **National Scholarship** under National Scholarship Scheme for B.Sc. (III year Hons.) Examination 2003 in Chemistry
16. **Certificate of Merit and National scholarship** from CBSE for being among top 0.1% students in All India Secondary School examination, 1998.

2025

1. Bhaskar Mondal, Luis R Domingo*, Haydar A Mohammad Salim, **Nivedita Acharjee*** (2025) Unveiling Intramolecular [3+2] Cycloaddition Reactions Leading to Functionalized Heterocycles in the Light of Molecular Electron Density Theory, *ChemPhysChem* (Wiley), e202401106, (IF:2.3) <https://doi.org/10.1002/cphc.202401106>
2. Barsali Banerjee, Luis R. Domingo, Haydar A. Mohammad-Salim, Asmita Mondal and **Nivedita Acharjee*** (2025) Understanding [3+2] cycloaddition reactions of difluoroallene to nitrene and diazoalkanes from the molecular electron density theory perspective, *New Journal of Chemistry (Royal Society of Chemistry)*, (IF:2.9) <https://doi.org/10.1039/D5NJ00464K>
3. Abdellatif Rafik, Hafid Zouihri, Hassna Jaber, Asmaa Oubihi, Abdellah Zeroual, Taoufiq Guedira, Kholood A. Dahlous, Mohammad Shahidul Islam, Nivedita Acharjee & Mohammed Salah (2025) Exploring hybrid phosphate compound $C_2H_6NO^+@H_2PO_4^-$: crystallography, optics, and bioactivity, *Chemical Papers (Springer)* (IF:2.1) <https://doi.org/10.1007/s11696-025-03927-7>

2024

4. Jamelah S Al-Otaibi, Y.Sheena Mary, Y.Shyma Mary, Asmita Mondal, Nivedita Acharjee, Deepthi S. Rajendran Nair (2024) Adsorption of toremifene on carboxylic acid functionalized N/B-doped coronene: DFT, AIM, Solvation, docking and MD analyses *Journal of Molecular Liquids* (Elsevier), 395, 123931 IF: 6.00 <https://doi.org/10.1016/j.molliq.2023.123931>
5. Aneesh Kumar R, Jamelah S. Al-Otaibi, Y. Sheena Mary, Y. Shyma Mary, Nivedita Acharjee, Renjith Thomas, Leena T L (2024) Surface adsorption of adenine on pristine and B/N/O/P-doped coronene as biosensing substrate for DNA detection- DFT Study. *Journal of Molecular Liquids* (Elsevier), 393, 123546 (IF: 6.00) <https://doi.org/10.1016/j.molliq.2023.123546>
6. Dr. Jamelah S Al-Otaibi, Y.Sheena Mary; Y.Shyma Mary; Asmita Mondal; Nivedita Acharjee; Deepthi S. Rajendran Nair (2024) Investigation of the interaction of thymine drugs with Be12O12 and Ca12O12 nanocages: a quantum chemical study, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (Elsevier), 308 (2024) 123728 (IF: 4.4) <https://doi.org/10.1016/j.saa.2023.123728>
7. Jamelah S. Al-Otaibi, Y. Sheena Mary, Asmita Mondal, Nivedita Acharjee, M.S. Roxy, H.S. Yathirajan, Maria Cristina Gamberini (2024) Understanding Trimipraminium Maleate (TPM) through Spectroscopic, Hirshfeld surface and reactivity analysis: Experimental, DFT and MD studies in different solvents at different temperatures, *Journal of the Indian Chemical Society* (Elsevier), Volume 101, Issue 10, October 2024, 101235; <https://doi.org/10.1016/j.jics.2024.101235> (IF = 3.20)
8. Bhaskar Mondal, Luis R. Domingo, Haydar A. Mohammad-Salim, Nivedita Acharjee (2024) Unveiling [3 + 2] cycloaddition reactions of diphenyl diazomethane to thiobenzophenone and cycloaliphatic thioketones in the light of molecular electron density theory, *Computational and Theoretical Chemistry* (Elsevier), 114660 (IF: 2.80) <https://doi.org/10.1016/j.comptc.2024.114660>
9. Amine Rafik, Hamza El Hadki, Abdeljabbar Jaddi, Najia Komiha, Oum Keltoum Kabbaj, Nivedita Acharjee, Mohammed Salah, Mohammad Azam, khadija Marakchi (2024) A new investigation into the regioselectivity and stereoselectivity of the reaction between di-methyl nitrene and fluorinated alkenes: DFT, independent gradient model, and molecular docking, *Computational and Theoretical Chemistry* (Elsevier), 1234, 114511 (IF: 2.80) <https://doi.org/10.1016/j.comptc.2024.114511>
10. Moulay Driss MELLAOUI, Khalid Abbiche, Nivedita Acharjee, Haydar Mohammad-Salim, Abdallah Imjjad, Rachid Boutiddar, Khadija Marakchi, Souad El Issami, Hanane Zejli (2024) Unveiling the mechanism and selectivity of the [3 + 2] cycloaddition reactions of nitrene with acetylene derivatives leading to anticancer 4-isoxazoline derivatives from the MEDT perspective, *Computational and Theoretical Chemistry* (Elsevier), 1237, 114619 (IF: 2.80), <https://doi.org/10.1016/j.comptc.2024.114619>
11. Haitham K.R. Al-Sharifi; Ani Deepthi; Nivedita Acharjee; M S Swapna; S. Sankararaman (2024) A Window to Energy Efficiency: Tryptanthrin-Malononitrile Knoevenagel Adduct as an IR Window Material, *Journal of Materials Science: Materials in Electronics* (Springer) (IF = 2.440) <https://doi.org/10.1007/s10854-024-13018-0>
12. Jamelah S Al-Otaibi, Fowzia S Alamro, Aljawhara H Almugrin, Y Sheena Mary, Nivedita Acharjee (2024) Adsorption, sensor properties, AIM analysis, docking of an anticancer drug benzamide on nanocones: SERS, solvent effects and DFT investigation, *Journal of Computational Biophysics and Chemistry* (World Scientific), (IF = 2.440) <https://doi.org/10.1142/S2737416524500091>

13. Abdellatif Rafik, Fatima Lakhdar, afid Zouihri, Taoufiq Guedira, Nivedita Acharjee, Mohammad Shahidul Islam, Mohammed Salah, Abdellah Zeroual (2024) Exploring nonlinear optical properties in a hybrid dihydrogen phosphate system: an experimental and theoretical approach, *Journal of Molecular Modeling* (Springer) (IF = 2.20) 30:151, <https://doi.org/10.1007/s00894-024-05936-x>
14. Asmita Mondal, Nivedita Acharjee*, Haydar Mohammad-Salim, Mrinmoy Chakraborty (2024) A Molecular Electron Density Theory Study to understand intramolecular [3+2] cycloaddition reactions of azides and diazoalkanes, *Structural Chemistry* (Springer), <https://doi.org/10.1007/s11224-023-02270-5> (IF = 1.795)
15. Mohammed Salah, Oumaima El Alaoui El Abdallaoui, Abdellah Zeroual, Nivedita Acharjee and Mohammed El idrissi (2024) Insight into a new discovery of SARS-CoV-2 inhibitor activated through Chloroquine derivatives, *Current Chemistry Letters*, 13(1), 49-60. <https://doi.org/10.5267/j.ccl.2023.8.010>
16. Asmita Mondal, Nivedita Acharjee* (2023) Unveiling the exclusive stereo- and site selectivity in [3+2] cycloaddition reactions of a tricyclic strained alkene with nitrile oxides from the molecular electron density theory perspective, *Chemistry of Heterocyclic Compounds Special Issue on "Cycloaddition reactions: Recent Progress (Springer)"* (IF = 1.490) <https://doi.org/10.1007/s10593-023-03176-0>
17. Asmita Mondal, Hayder A Mohammad-Salim, Nivedita Acharjee* (2023), Unveiling substituent effects in [3+2] cycloaddition reactions of benzonitrile N-oxide and benzylideneanilines from the molecular electron density theory perspective, *Scientific Radices*, Volume 2, page-88-105, <https://doi.org/10.58332/scirad2023v2i1a05>

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18. Jamelah S Al-Otaibi, Y.Sheena Mary, Y.Shyma Mary, **Nivedita Acharjee**, Deepthi S. Rajendran Nair, Yathirajan HS (2023) An investigation on spectroscopic, wavefunction dependent reactivity, docking and anti-Covid-19 ability of Flupentixol dihydrochloride: DFT and MD simulations at different temperatures, *Journal of Molecular Liquids (Elsevier)*, 392, 123177 (IF: 6.00) <https://doi.org/10.1016/j.molliq.2023.123177>
19. Luis R Domingo*, **Nivedita Acharjee**, (2023) " Unveiling the Mg(II) Promoted [3+2] Cycloaddition Reaction of Mesitonitrile Oxide to Baylis-Hilman Adduct from the Molecular Electron Density Theory Perspective", *New Journal of Chemistry (Royal Society of Chemistry)*, 47, 2495-2506 (IF = 3.925) <https://doi.org/10.1039/D2NJ05424H>
20. Jamelah S.Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, **Nivedita Acharjee**, Sreejit Soman (2023) Spectroscopic, reactivity analysis and docking studies of 3-(adamantan-1-yl)-4-(4-fluorophenyl)-1-[(4-phenylpiperazin-1-yl)methyl]-4,5-dihydro-1H-1,2,4-triazole—5-thione: DFT and MD simulations, *Journal of Molecular Structure (Elsevier)*, 134418. (IF = 3.841) <https://doi.org/10.1016/j.molstruc.2022.134418>
21. Jamelah S. Al-Otaibi, Y.Sheena Mary, Y.Shyma Mary, Asmita Mondal, Nivedita Acharjee, Jineet kumar Gawad, Insights on adsorption properties of a DNA base, guanine on nano metal cages (Ag₂₄/Au₂₄/Cu₂₄): DFT, SERS, NCI and solvent effects, *Journal of Molecular Structure (Elsevier)*, 135541. (IF = 3.841) <https://doi.org/10.1016/j.molstruc.2023.135541>
22. P. Vennila, Jamelah S. Al-Otaibi, G. Venkatesh, Y. Sheena Mary, V. Raj, **Nivedita Acharjee** & P. Tamilselvi (2023): Structural, Spectral, Molecular Docking, and Molecular Dynamics Simulations of Phenylthiophene-2-Carboxylate Compounds as Potential Anticancer Agents, *Polycyclic Aromatic Compounds (Taylor and Francis)* (IF = 3.744) <https://doi.org/10.1080/10406638.2023.2172052>
23. A. Khannous a, S. Jorio, **N. Acharjee**, M. Azam, K. Min, M. Salah (2023) Unveiling the atropoisomerism induced facial selectivity and regioselectivity in the [3 + 2] cycloaddition reaction of benzonitrile oxide with 5-methylenehydantoin from the molecular electron density theory perspective, *Computational and Theoretical Chemistry (Elsevier)*, Volume 1227, September 2023, 114243 (IF = 2.800) <https://doi.org/10.1016/j.comptc.2023.114243>
24. Bhaskar Mondal; Luis R. Domingo; Haydar A. Mohammad-Salim; **Nivedita Acharjee*** (2023), Unveiling the mechanism, regiochemistry and substituent effects of the [3+2] cycloaddition reactions of C, N-diaryl nitrile imine to ethylene derivatives from the molecular electron density theory perspective, *Computational and Theoretical Chemistry (Elsevier)* <https://doi.org/10.1016/j.comptc.2023.114393> (IF = 2.800)
25. Jamelah S Al-Otaibi*, Y.Sheena Mary, Y.Shyma Mary, **Nivedita Acharjee**, Abdulaziz A. Al-Saadi, Maria Cristina Gamberini (2023) Influence of pyramidal M₂₀ (M=Cu, Ag, Au) clusters on SERS and non-covalent interactions towards tuberculosis drug Pretomanid (PTD): DFT study, *Journal of Computational Biophysics and Chemistry* (accepted) (IF = 2.440)
26. Moulay Driss Mellaoui, **Nivedita Acharjee***, Abdallah Imjjad, Jamal Koubachi, Abdellatif El Hammadi, Hassan Bourzi, Souad El Issami, Hanane Zejli, Majdi Hochlaf*, and Khalid Abbiche* (2023) Unveiling the mechanism, selectivity, solvent and temperature effects on the [3+2] cycloaddition reaction of N-methyl-C-(2-furyl) nitron with maleimide derivatives from the molecular electron density theory perspective, *Theoretical Chemistry Accounts (Springer)*, 142, 33 (IF = 1.700) <https://doi.org/10.1007/s00214-023-02972-3>

27. Asmita Mondal, Luis R Domingo, **Nivedita Acharjee*** (2023) Revealing the influence of tether length on the intramolecular [3+2] cycloaddition reactions of nitrones from the molecular electron density theory perspective, *Journal of Physical Organic Chemistry (Wiley)* (**IF: 1.800**). <https://doi.org/10.1002/poc.4574>
28. Barsali Banerjee, **Nivedita Acharjee***, Debnath Palit (2023) Revealing the cyclization selectivity in intramolecular [3+2] cycloaddition reactions of allenic nitrones from the molecular electron density theory perspective, *Structural Chemistry (Springer)*, (**IF = 1.795**) <https://doi.org/10.1007/s11224-023-02175-3>
29. Asmita Mondal, **Nivedita Acharjee***, Debnath Palit (2023) Unveiling [3+2] cycloaddition reactions of pyridinium bis(methoxycarbonyl)methylides and pyridinium dicyanomethylides with cyclooctyne for indolizine synthesis from the molecular electron density theory perspective, *Structural Chemistry (Springer)*, (**IF = 1.795**) <https://doi.org/10.1007/s11224-023-02193-1>
30. Haydar Mohammad-Salim, Asmita Mondal, Jesus Vicente de Julián-Ortiz, **Nivedita Acharjee** (2023), Diastereoselective green synthesis of pyrrolo[1,2-a]quinolines via [3+2] cycloaddition reaction: insights from molecular electron density theory, *Theoretical Chemistry Account (Springer)*, 142, 129, (**IF:1.7**), <https://doi.org/10.1007/s00214-023-03068-8>

2022

31. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, Asmita Mondal, **Nivedita Acharjee**, S. Balachandar (2022) Investigation of the adsorption of a DNA based purine derivative on N/B-doped coronene and coronene by means of DFT and NCI interaction analysis, *Journal of Molecular Liquids (Elsevier)*, 367, 120373 (**IF = 6.633**) <https://doi.org/10.1016/j.molliq.2022.120373>
32. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, **Nivedita Acharjee**, S. Balachandar, H.S. Yathirajan (2022), Insights into solvation effects, spectroscopic, Hirshfeld Surface Analysis, reactivity analysis and anti-Covid-19 ability of doxylamine succinate: Experimental, DFT, MD and docking simulations, *Journal of Molecular Liquids (Elsevier)*, 361, 119609 (**IF = 6.633**) <https://doi.org/10.1016/j.molliq.2022.119609>
33. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, Asmita Mondal, **Nivedita Acharjee** (2022) DFT analysis on the adsorption of melamine in Ga12-N12/P12 nanocages: solvent effects, SERS analysis, reactivity properties, *Journal of Biomolecular Structure and Dynamics (Taylor and Francis)* (**IF = 5.235**) <https://doi.org/10.1080/07391102.2022.2137700>
34. **Nivedita Acharjee***, Asmita Mondal, Mrinmoy Chakraborty (2022) "Unveiling intramolecular [3+2] cycloaddition reactions of C, N-disubstituted nitrones with a molecular electron density theory perspective", *New Journal of Chemistry (Royal Society of Chemistry)*, 2022, 46, 7721-7735 (**IF = 3.925**) <https://doi.org/10.1039/d2nj00888b>
35. Luis R Domingo*, Mar-Rioz Gutiérrez, **Nivedita Acharjee** (2022) "A Molecular Electron Density Theory Study of the Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Nitrones with Nucleophilic Ethylenes", *European Journal of Organic Chemistry (Wiley)* 2022, e202101417 (**IF = 3.261**) <https://doi.org/10.1002/ejoc.202101417>
36. Luis R. Domingo*, Mar Ríos-Gutiérrez, **Nivedita Acharjee** (2022) "Unveiling the cb-type Intramolecular [3+2] Cycloaddition Reactions of Fluorinated Azomethine Ylides to Ester Carbonyls with a Molecular Electron Density Theory Perspective", *ChemistrySelect (Wiley)*, 7, e202201845 (**IF = 2.307**) <https://doi.org/10.1002/slct.202201845>
37. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, Sreejit Soman, **Nivedita Acharjee**, B. Narayana (2022), Theoretical and experimental investigation of a pyrazole derivative- solvation effects, reactivity analysis and MD simulations, *Chemical Physics Letters (Elsevier)*, 139469. (**IF = 2.719**) <https://doi.org/10.1016/j.cplett.2022.139469>
38. Ani Deepthi, **Nivedita Acharjee**, Sruthi S. L., Meenakshy C. B (2022) An overview of nitrile imine based [3+2] cycloadditions over half a decade, *Tetrahedron (Elsevier)*, 116, 132812 (**IF = 2.388**) <https://doi.org/10.1016/j.tet.2022.132812>
39. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, **Nivedita Acharjee**, David G. Churchill (2022), Spectroscopic studies of 5-fluoro-1H-pyrimidine-2,4-dione adsorption on nanorings, solvent effects and SERS analysis, *Computational and Theoretical Chemistry (Elsevier)*, (**IF = 2.292**) <https://doi.org/10.1016/j.comptc.2022.113873>
40. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, Asmita Mondal, **Nivedita Acharjee**, David G. Churchill (2022), Sumanene as a delivery carrier for methimazole drug: DFT, AIM, SERS and solvent effects, *Computational and Theoretical Chemistry (Elsevier)*, 1215, 113811 (**IF = 2.292**) <https://doi.org/10.1016/j.comptc.2022.113811>

41. Jamelah S. Al-Otaibi, Y. Sheena Mary*, Y. Shyma Mary, **Nivedita Acharjee** (2022) Quantum mechanical investigation into the adsorption pattern of clomipramine and methotrimeprazine HCl with graphene and fullerene, *Polycyclic Aromatic Hydrocarbons (Taylor and Francis)* (IF = 2.195)
<https://doi.org/10.1080/10406638.2022.2041678>
42. Said Kerraj, Mohammed Salah*, Samir Chtita, Mohammed El Idrissi, Said Belaouad, Moutaabid Mohammed, **Nivedita Acharjee**, Najia Komaha (2022), Theoretical study of photovoltaic performances of Ru, Rh and Ir half sandwich complexes containing N,N chelating ligands in Dye- Sensitized Solar Cells (DSSCs). DFT and TD-DFT investigation, *Computational and Theoretical Chemistry (Elsevier)*, 1209, 113630 (IF = 2.292) <https://doi.org/10.1016/j.comptc.2022.113630>
43. **Nivedita Acharjee***, H. A. M. Salim, Mrinmoy Chakraborty (2022) "Unveiling the synthesis of spirocyclic, tricyclic and bicyclic triazolooxazines from intramolecular [3+2] azide-alkyne cycloadditions with a molecular electron density theory perspective", *Structural Chemistry (Springer)*, 33, 555-570 (IF = 1.795)
<https://doi.org/10.1007/s11224-021-01870-3>
44. **Nivedita Acharjee***, H. A. M. Salim, Mrinmoy Chakraborty (2022) "Unveiling the regioselective synthesis of antiviral 5-isoxazol-5-yl-2' deoxyuridines with a molecular electron density theory perspective", *Journal of the Serbian Chemical Society*, 87, 707-721 (IF = 1.240)
<https://doi.org/10.2298/JSC211014106A>
45. Ali Barhoumi, Mohammed Salah, Abdallah Zeroual, Mrinmoy Chakraborty, **Nivedita Acharjee*** (2022), Unveiling the reactions of triethylphosphite and its diethylamino substituted derivatives to carbon tetrachloride with a molecular electron density theory perspective, *Indian Journal of Chemistry*, 61, 127-135. <http://op.niscpr.res.in/index.php/IJC/article/view/60707>
46. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, **Nivedita Acharjee**, D. G. Churchill (2023) Theoretical study of Glycoluril by highly symmetrical magnesium oxide Mg₁₂O₁₂ nanostructure: Adsorption, Detection, SERS enhancement and electrical conductivity study, *Journal of Molecular Modeling (Springer)* 28, 332 (IF = 2.172)
47. Jamelah S. Al-Otaibi*, Y. Sheena Mary, Y. Shyma Mary, **Nivedita Acharjee**, Zakir Ullah (2022) DFT, solvation effects, reactivity and SERS analysis on structural, optical, and vibrational properties of a biomolecule of pyrimidine derivative adsorbed on metal clusters of Ag/Au/Cu, *Journal of the Indian Chemical Society (Elsevier)*, 99, 100753, <https://doi.org/10.1016/j.jics.2022.100753>

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48. Luis R Domingo*, **Nivedita Acharjee** (2021), Unveiling the Substituent Effects in the Stereochemistry of [3+2] Cycloaddition Reactions of Aryl- and Alkyldiazomethylphosphonates with Norbornadiene within a MEDT Perspective, *ChemistrySelect (Wiley)*, 6, 10722-10733 (IF = 2.109)
<http://dx.doi.org/10.1002/slct.202102942>
49. **Nivedita Acharjee***, H. A. M. Salim, Mrinmoy Chakraborty (2021) Unveiling [3+2] cycloaddition reactions of benzonitrile oxide and diphenyl diazomethane to cyclopentene and norbornene: A molecular electron density theory perspective, *Theoretical Chemistry Accounts (Springer)*, 140, 113 (IF = 1.702).
<https://doi.org/10.1007/s00214-021-02811-3>
50. Luis R. Domingo*, **Nivedita Acharjee*** (2021) Unveiling the Chemo- and Regioselectivity of the [3+2] Cycloaddition Reaction between 4-Chlorobenzonitrile Oxide and β-Aminocinnamonitrile with a MEDT Perspective, *ChemistrySelect (Wiley)*, 6, 4521-4532 (IF = 2.109) (**Top downloaded paper of 2021 - 2022 recognized by Wiley**) <https://doi.org/10.1002/slct.202100978>
51. **Nivedita Acharjee***, H. A. M. Salim, Mrinmoy Chakraborty, Madhuri P Rao, Madhu Ganesh (2021) Unveiling the high regioselectivity and stereoselectivity within the synthesis of spirooxindolenitropyrrolidine: A molecular electron density theory perspective, *Journal of Physical Organic Chemistry (Wiley)*, e4189 (IF = 2.391) (**Top cited paper of 2021-2022 recognized by Wiley**) <https://doi.org/10.1002/poc.4189>
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<https://doi.org/10.1007/s00214-020-02703-y>
55. Luis R. Domingo *, Mar Ríos-Gutiérrez, **Nivedita Acharjee** (2021) Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory, *Chemistry (MDPI)*, 3(1), 74-93.
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80. **Nivedita Acharjee**, Avijit Banerji*, Biswajit Gayen (2011), Cycloaddition approach to five- membered heterocycles – Some recent experimental and theoretical aspects. Invited Review on 150th Birth anniversary Commemoration of Acharya Prafulla Chandra Ray, *Journal of the Indian Chemical Society*, 88, 1857.
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Book Chapter

87. Luis R Domingo*, **Nivedita Acharjee** (2020), Molecular Electron Density Theory-A New Theoretical Outlook on Organic Chemistry *Frontiers in Computational Chemistry-Volume 5*, Published by Bentham and Science Pvt. Ltd. <https://doi.org/10.2174/9789811457791120050007>

Research Articles in Edited Volumes

88. **Mandal S, Acharjee N***, Chakraborty B —DFT studies for generation of stereospecific antibacterial cycloadduct from symmetrically substituted reactant. I., —Chemistry on its Way-Impacts on the Environment I, (Ed: Samiran Mandal), Saldiha College (ISBN : 978-93-84191-17-7); [**Published in 2017**]
89. **Mandal S, Acharjee N***, Banerji A, —Conceptual DFT interpretations for diastereoselective synthesis of tetrasubstituted isoxazoidines I, (Ed: Kamala Mitra) Dept. of Chemistry, Prasanta Chandra Mahalanobish Mahavidyalaya (ISBN : 978-93-8310-31-8) [**Published in 2017**]

General Articles/Periodicals

90. Asmita Mondal, Avijit Banerjee*, **Nivedita Acharjee** (2022) Understanding [3+2] cycloaddition reactions from the molecular electron density perspective: A new theoretical outlook on organic reactions, *Edu. Chem. Sci. Tech.*, Vol 10, August 2022 (Periodical published by the Indian Chemical Society)
91. **Nivedita Acharjee** (2019): Impact of solar radiation on human health, *CURE (Congregation for Urban and Rural Environment)*, *Environmental Bulletin 2019, Volume XXV, ISSN: 2319-1333*
92. **Nivedita Acharjee** (2019): Beauty of "Golden Ratio" in paintings, architecture, music, nature and technology, *Communique*, Academic Journal of Durgapur Government College, *ISSN No. 0973-8584*.
93. **Nivedita Acharjee*** (2018), Impact of smog on public health, *CURE (Congregation for Urban and Rural Environment)*, *Environmental Bulletin 2018, Volume XXIV, ISSN: 2319-1333*
94. **Nivedita Acharjee*** (2018), —Scientific Story of our laughter, crying and stress I: *Everyman's Science*, Journal published by Indian Science Congress Association, *ISSN: 0531-495X*
95. **Nivedita Acharjee*** (2017), The Scientific Face of our emotions, *Communique*, Academic Journal of Durgapur Government College, *ISSN No. 0973-8584*.
96. **Nivedita Acharjee*** (2017), Effect of particulate matter on Human Health and Environment, *CURE (Congregation for Urban and Rural Environment)*, *Environmental Bulletin 2017, Volume XXIII, ISSN: 2319-1333*
97. **Nivedita Acharjee*** (2015), "Molecular Processes of Aging": Vol. XXI, *Environmental Bulletin 2015, CURE (Congregation for urban and rural environment)*, *ISSN: 2319-1333*
98. **Nivedita Acharjee*** (2014), —The Aging Process: Accelerators and Decelerators I: Aug 13- Sep 13 issue, *Everyman's Science*, Journal published by Indian Science Congress association, *ISSN: 0531-495X*

Sponsored Projects

1. **Dr. Nivedita Acharjee**, Coordinator, DBT STAR COLLEGE SCHEME for Durgapur Government College sponsored by Department of Biotechnology, Government of India, Project No. HRD-11011/24/2022-HRD-DBT dated 29-09-2022 (Period: 29-09-2022 to 28-09-2025)] (Rs. 120.38469 Lakhs)
2. **Dr. Nivedita Acharjee** (PI), UGC Minor research Project No. F. PSW-111/11-12 (ERO) "Experimental and theoretical DFT investigations of the effects of mild Lewis acid catalysts on the cycloaddition reactions of acyclic and cyclic aldonitrone to α,β -unsaturated ketones and esters" (Period: 8.11.2011 to 7.11.2013)] (Rs. 1.35 Lakhs)

Guidance of Ph.D. Scholar and M.Sc. Project Dissertations

1. Asmita Mondal (2022, *Durgapur Government College*) [enrolled for Ph.D.]
2. Barsali Banerji (2023, *Durgapur Government College*) [enrolled for Ph.D.]
3. Bhaskar Mondal (2023, *Durgapur Government College*) [enrolled for Ph.D.]
4. Mousmi Narayan Kar (2024, *Durgapur Government College*) Studying the Bioactivity of Diphenylamine, Bromelain and citric acid through computation. [M.Sc.]
5. Somali Goswami (2024, *Durgapur Government College*) Studying the Bioactivity of Piperine, Curcumin & Capsaicin through Computation [M.Sc.]
6. Soubhik Chakraborty (2023, *Durgapur Government College*) N-t-Butyl- aryl Nitrones as Potent Spin Traps: DFT Analysis of Electron Localization Function Topology, Local Selectivity, Reactivity and Solvent Effects [M.Sc.]
7. Sangram Singh (2023) DFT Calculations for the Analysis of Selectivity, Reactivity and Solvent Effects of 5,5-Dimethyl-1-Pyrroline-N-Oxide (DMPO) Nitrones Towards Radical Capture) As Spin Traps) [M.Sc.]
8. Shreyasee Nath (2022, *Durgapur Government College*) DFT calculations for the
9. analysis of frontier molecular orbitals and reactivity indices of tricyclic pyrrolidine - fused benzo[b] thiophene 1, 1 - dioxide(M. Sc.) Subarna Khan (2021, *Durgapur Government College*): Energy profile study associated with the[3+2] cycloaddition reaction of 1-pyrroline-1-oxide with nvinyl nucleobases[M.Sc.]
10. Asmita Mondal (2020, *Durgapur Government College*): Chemical profiling and theoretical analysis of polysaccharides in rice bran [M.Sc.]
11. Sourav Mondal (2019, *Durgapur Government College*): Solvent effects on [3+2] cycloaddition reactions of N-tert-butylmethanimine-N-oxide [M.Sc.]
12. Monirul Islam (2019, *Durgapur Government College*); 1,3-dipolar cycloaddition reactions: classification, selectivity and catalysis [M.Sc.]
13. Mira Jhawar (2018, *Durgapur Government College*): Allyl type 1,3-dipoles: DFT study augmented with ELF topological analysis [M.Sc.]
14. Ambar Barman (2018, *Durgapur Government College*): Allenyl type 1,3-dipoles: DFT study augmented with ELF topological analysis [M.Sc.]
15. Suranjana Sen (2017, *Durgapur Government College*): Experimental and Theoretical Studies On Synthesis and Spectroscopy of C-(4-chlorophenyl)-N-phenyl nitrone [M.Sc.]
16. Jayanta Mondal (2017, *Durgapur Government College*): Synthesis, global properties and vibrational analysis of C-(4-bromophenyl)-N-phenyl nitrone [M.Sc.]
17. Nasrin Jahan (2017, *Durgapur Government College*): Synthesis, vibrational analysis and cycloaddition reactions of chalcone to C-aryl-N-phenyl nitrones :Experimental and theoretical studies [M.Sc.]
18. Akash Mitra (2016, *Durgapur Government College*): Effect of substituents on the frontier molecular orbital energies and global properties of Isoxazolidines: AM1 study [M.Sc.]

Invited Lectures

1. "**How to develop and upload and upload E-content in 4 quadrants?**"; Workshop organized by Internal Quality Assurance Cell, Durgapur Government College on March 14, **2019**
2. "**Career Counselling and Placement after Secondary and Senior Secondary level**"; Special Programme organized by Assembly of God Church School, Okhra, West Bengal on 1st November **2017**.
3. "**Gender Equality for Sustainable Development**"; NSS Special Camp, Organized by NSS Unit, Durgapur Government College in **2016**
4. "**Gender Equality: Indispensable yet overlooked**"; Awareness Programme on International Women's Day; organized by Cell for Gender Sensitization and Protection of Sexual Harassment against Women, Durgapur Government College on 8th March **2016**.

Abstracts in seminar/conference

1. 2ND INTERNATIONAL CONFERENCE ON EMERGING AREAS OF CHEMISTRY (ICEAC) held at Tripura University, Agartala from 12th to 14th February, 2025, Paper entitled "QTAIM and ELF analysis for adsorption of toremifene and DNA-based purine on N/B doped coronene" *Oral Presentation by PhD student Asmita Mondal*
2. 2ND INTERNATIONAL CONFERENCE ON EMERGING AREAS OF CHEMISTRY (ICEAC) held at Tripura University, Agartala from 12th to 14th February, 2025, Paper entitled "Unveiling the [3+2] Cycloaddition Reactions of 1,1-Difluoroallene to Nitron and Diazoalkane: A Density Functional Theory Study" *Oral Presentation by PhD student Barsali Banerjee.*
3. ICBS-2025, held at Surendranath College, Kolkata on 3rd January, 2025, Paper entitled "QTAIM and MEP analysis of sumanene as a delivery carrier for methimazole drug" *Poster Presentation by PhD student Asmita Mondal*
4. ICBS-2025, held at Surendranath College, Kolkata on 3rd January, 2025, Paper entitled "Density Functional Theory analysis for intramolecular and intermolecular versions of nitron-allene addition in [3+2] cycloaddition reactions" *Poster Presented by PhD student Barsali Banerjee.*
5. ICBS-2025, held at Surendranath College, Kolkata on 3rd January, 2025, Poster entitled "Density Functional Theory (DFT) analysis to understand the electronic structure of Chrysin, a promising natural flavonoid and polyphenol" *Poster Presentation by B.Sc. student Sneha Mondal*
6. ICBS-2025, held at Surendranath College, Kolkata on 3rd January, 2025, Poster entitled "A computational DFT Study to comprehend the electronic structure of Rosmarinic Acid" *Poster Presentation by B.Sc. student Rajashree Maji*
7. ICBS-2025, held at Surendranath College, Kolkata on 3rd January, 2025, Poster entitled "Density Functional Theory Modeling of L-citrulline in terms of FMO theory and electron localization function (ELF) analysis" *Poster Presentation by B.Sc. student Bishnupriya Pal and won the best poster award under student category.*
8. ACS-CRSI Early Career Researchers' Symposium 2024, held at KIIT University, Bhubaneswar from 22nd to 23rd October 2024, Paper entitled "Unveiling Water Mediated Green Synthesis of pyrrolo[1,2-a]quinolines in the light of Density Functional Theory" *Poster and Oral Presentation by PhD student Asmita Mondal.*
9. International Conference on Natural Sciences and Engineering for Sustainable Development organized by Centre for Organic Spintronics and Optoelectronic Devices in collaboration with Department of Physics, Kazi Nazrul University from **March 06-07, 2024**. Paper entitled, "Understanding intramolecular [3+2] cycloaddition reactions of allenic nitrones in the light of Molecular Electron Density Theory" *Presented by PhD student Barsali Banerjee.*
10. International Conference on Natural Sciences and Engineering for Sustainable Development organized by Centre for Organic Spintronics and Optoelectronic Devices in collaboration with Department of Physics, Kazi Nazrul University from **March 06-07, 2024**. Paper entitled, "A Quantum Chemical study for [3+2] cycloaddition reactions of C,N-diaryl imine with ethylene derivatives from the molecular electron density theory perspective" *Presented by PhD student Bhaskar Mondal.*
11. 28th ISCB International Conference (ISCBC-2024). Held at Marwadi University, Rajkot, Gujarat from 8th to 10th January 2024, a Paper entitled "Understanding indolizine synthesis from [3+2] cycloaddition reactions of substituted pyridinium methylides with molecular electron density theory perspective" *Presented by PhD student Asmita Mondal.*
12. 27th ISCB International Conference (ISCBC-2022). Held at Birla Institute of Technology, Mesra, Ranchi from 16th to 19th November 2022, a Paper entitled "Unveiling the synthesis of isoxazolidines from intramolecular [3+2] nitron cycloadditions in terms of molecular electron density theory" *Presented by PhD student Asmita Mondal.*
13. Equinox 2022, The Annual International Conference on the occasion of celebrating Century Year of University of Delhi, Paper entitled "Unveiling [3+2] Cycloaddition Reactions from the Molecular Electron Density Theory Perspective", **August 11-13, 2022**, *Presented by PhD student Asmita Mondal.*
14. International Seminar on Recent Advances in Chemistry and Material Science (RACMS-2022) on the occasion of 161st Birth Anniversary Celebration of Acharya P. C. Ray, Paper entitled "Unveiling the mechanism and substituent effects in the synthesis of fused tricyclic 1,2,3-triazolines and 1,2,3-triazoles from intramolecular [3+2] cycloadditions within the molecular electron density theory framework", **July 30-31, 2022**, *Presented by PhD student Asmita Mondal.*
15. International Research Scholars' meet on the occasion of 99th Foundation Day celebration of Indian Chemical Society, Paper entitled "Unveiling intramolecular [3+2] cycloaddition reactions of nitrones and azides from the molecular electron density theory perspective", **May 9, 2022**, *Presented by PhD student Asmita Mondal and received award of excellence.*
16. International Seminar on "Advancements in Chemical Sciences: Issues and Challenges", organized by Asansol B.B. College, Asansol, **February 4-5, 2020**. Paper entitled: Molecular electron density theory study to analyse [3+2] cycloaddition reactions leading to biologically active five-membered heterocycles", *Presented by Dr. Nivedita Acharjee*
17. International Seminar on "Innovation, Expansion, Impacts and Challenges in Chemical and Biological Sciences" organized by Surendranath College, Kolkata, **January 8-9, 2020**, Paper entitled: N-t-butyl- α -aryl nitrones as potent spin traps of biologically relevant free radicals: DFT analysis of electron localization function topology, local selectivity, reactivity, and solvent effects", *Presented by Sourav Mondal (M.Sc. Student)*
18. International Seminar on "Innovation, Expansion, Impacts and Challenges in Chemical and Biological Sciences" organized by Surendranath College, Kolkata, **January 8-9, 2020**, Paper entitled: Understanding the chemo-, regio and stereoselective synthesis of an anticancer spiroisoxazoline derived from α -santonin in the light of molecular electron density theory", *Presented by Nivedita Acharjee*

19. National Seminar on "Modern Era of Biosciences: Lab to land" organized by Departments of Conservation Biology and Zoology, Durgapur Government College, **December 05, 2019**, Paper entitled: *DFT study of the Electronic Structure and Reactivity of the Nitron moiety as potent radical spin trap for hydroxyl radical to fight the aging process*", Presented by Nivedita Acharjee
20. National Seminar on Chemistry for Sustainable Development organized by Sidho-Kanho-Birsha University in collaboration with Indian Chemical Society; during **November 26-27, 2019**, Paper entitled: *"DFT study of the selectivity and reactivity of potent radical spin trap N-t-butyl- α - phenyl nitron (PBN) in terms of global & local indices and electron localization function topological analysis"*, Presented by Sourav Mondal (M.Sc. Student).
21. DAE and CSIR sponsored International Level Conference on "Non-linear Dynamics and its applications" during **March 12-14, 2019** at Dept. of Physics, Durgapur Government College; Paper entitled "Understanding the pathway of [3 + 2] cycloaddition reactions of C-phenyl-N- methyl nitron in terms of BET (Bonding Evolution Theory) and QTAIM (Quantum Theory of atoms in Molecules) analyses", Presented by Nivedita Acharjee
22. DAE and CSIR sponsored International Level Conference on "Non-linear Dynamics and its applications" during **March 12-14, 2019** at Dept. of Physics, Durgapur Government College; Paper entitled "Molecular Electron Density Theory: A computational chemistry approach to understand the reactivity of organic reactions", Presented by Nivedita Acharjee
23. DST, DRDO and DAE sponsored National Level Seminar on "Non-linear Dynamics and its applications" during **February 7-9, 2017** at Dept. of Physics, Durgapur Government College; Paper entitled "Density Functional Theory applications for interpretations of chemical reactions", Presented by Nivedita Acharjee
24. UGC sponsored National Level Seminar on "Modern Trends in Chemical Sciences" during **November 25-26, 2016** at Dept. of Chemistry, Prasanta Chandra Mahalanobish Mahavidyalaya ; Paper entitled "DFT Study for nitron cycloadditions to benzylidene acetone in terms of reactivity indices, interaction energies and activation parameters", Presented by Nivedita Acharjee (Awarded best poster presentation)
25. UGC Sponsored National Seminar on "A Journey Through Recent Developments In Chemistry" organized jointly by Department of Chemistry, Acharya B. N. Seal College Cooch Behar, West Bengal and Department of Chemistry, University of North Bengal, Darjeeling, West Bengal, **March 1st and 2nd 2012**; Paper entitled "Accelerative and stereoselective influence of mild Lewis acid coordination in dipolar cycloadditions: Experimental and DFT study", Presented by Nivedita Acharjee
26. Chemical Research Society of India Eastern Zonal Meeting 2011 and Celebration of the International Year of Chemistry 2011, **July 22-24, 2011**; Poster no. 4, Page: 22, organized by Department of Chemistry, University of North Bengal, Darjeeling, West Bengal; Paper Entitled "DFT study evidenced by X-Ray and NMR analysis for the cycloaddition reactions of C,N disubstituted aldonitrones in terms of reactivity indices, interaction energies and activation parameters", Presented by Nivedita Acharjee
 2nd UGC sponsored National seminar on advanced spectroscopy, theoretical chemistry, synthesis, reactivity and structure evaluation, organized by University of Burdwan, Burdwan, 20-22nd February **2009**; Paper entitled: "Studies on Nitron Cycloadditions to α , β - unsaturated ketones" (Awarded best oral presentation in organic chemistry); Presented by Nivedita Acharjee
27. 45th Annual convention of chemists **2008**; Paper entitled "Systematic spectroscopic investigations of C-aryl- N-methyl nitrones" Presented by Nivedita Acharjee
 Symposium on "Acharya Prafulla Chandra Ray and Chemistry Today" organized jointly by Indian Chemical Society and Department of Chemistry, University of Calcutta, **2007**; Paper entitled "A cycloaddition approach to masked triketomethanes" Presented by Nivedita Acharjee