

RESEARCH PUBLICATIONS IN INTERNATIONAL JOURNALS

2026

1. Jamelah S. Al-Otaibi, Y. Sheena Mary, Martin Krátký, Jarmila Vinsova, **Nivedita Acharjee**, Maria Cristina Gamberini (2026) SERS spectra, AIM, and MD investigations of a bioactive acetamide, an AChE and BChE inhibitor derivative, *Journal of Nanoparticle Research*, (Springer), Volume 28, 18 (IF: 2.5), <https://doi.org/10.1007/s11051-025-06538-1>
2. Jamelah S. Al-Otaibi, Fowzia S. Alamro, Aljawhara H. Almugrin, Y. Sheena Mary, Asmita Mondal, **Nivedita Acharjee**, Maria Cristina Gamberini (2026) Adsorption and electronic interactions of glycine on Al₁₂N₁₂ & B₁₂N₁₂ nanocages: a DFT study, *Journal of Molecular Liquids* (Elsevier), 447 (2026) 129373 (IF: 5.2) <https://doi.org/10.1016/j.molliq.2026.129373>
3. Bhaskar Mondal, Luis R Domingo*, Haydar A Mohammad Salim, **Nivedita Acharjee*** (2026) Understanding the domino reaction of aryl nitrilimine with quinoxaline in the light of molecular electron density theory, *Chemistry of Heterocyclic Compounds* (Springer) (Accepted)
4. Barsali Banerjee, Luis R Domingo*, Haydar A Mohammad Salim, **Nivedita Acharjee*** (2026) Unveiling the Synthesis of Spiroheterocycles from the [3+2] Cycloaddition Reactions of Oxadiazol-imine with Nitrile Oxide and Nitrile Imine in the Light of Molecular Electron Density Theory, *Chemistry of Heterocyclic Compounds* (Springer) (minor revision submitted)

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5. Abderrahmane Elmelouky, Hairch Youssef, Kholood A. Dahlous, Mohammad Shahidul Islam, **Nivedita Acharjee**, Mohammed Salah, Ahmed Mohamed Tawfeek (2025) Exploring dielectric relaxation and AC conductivity of layered double hydroxides, *Journal of Computational Electronics* (Springer), Volume 24, 164 (IF: 2.5), <https://doi.org/10.1007/s10825-025-02401-7>
6. Jamelah S. Al-Otaibi, Y. Sheena Mary, Asmita Mondal, **Nivedita Acharjee**, and Maria Cristina Gamberini (2025) Computational Insight into the Non-Covalent Binding of Amiloride with Sumanene: A DFT and QTAIM Perspective, *Chemistry Select* (Wiley), Volume 10, e03215 (IF:2). <https://doi.org/10.1002/slct.202503215>
7. Asmita Mondal, Luis R. Domingo, Haydar A. Mohammad-Salim, **Nivedita Acharjee** (2025) A Molecular Electron Density Theory Study for the Synthesis of Spirocyclic and Tricyclic Isoxazolines and Their Molecular Docking Evaluation for Antituberculosis Activity, *Journal of Physical Organic Chemistry* (Wiley), Volume 38, Issue 8, 2025, e70028 (IF:2.3); <https://doi.org/10.1002/poc.70028>
8. Jamelah S. Al-Otaibi, Y. Sheena Mary, **Nivedita Acharjee**, Ravi Kumar Trivedi, Brahmananda Chakraborty, M.S. Roxy (2025) DFT investigations of therapeutic competence of B₃O₃ as an efficient drug delivery agent for phosphonoacetic acid (PAA) antiviral drug, *Computational and Theoretical Chemistry* (Elsevier), Volume 1252, 115406; <https://doi.org/10.1016/j.comptc.2025.115406>
9. Sahil, Asmita Mondal, **Nivedita Acharjee**, Dilbag Singh, Neeraj Gupta (2025); Computational and Experimental Studies on Mixed-Phase Copper Species Deposited on Nitrogen-Doped Carbon Nanofibers for Electrochemical Sensing of Norfloxacin, *Electroanalysis* (Wiley), Volume 37, Issue 7, July 2025, e70001; <https://doi.org/10.1002/elan.70001> (IF:2.3)
10. 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>
11. Barsali Banerjee, Luis R. Domingo, Haydar A. Mohammad-Salim, Asmita Mondal and **Nivedita Acharjee*** (2025) Understanding [3+2] cycloaddition reactions of difluoroallene to nitron and diazoalkanes from the molecular electron density theory perspective, *New Journal of Chemistry*

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<https://doi.org/10.1039/D5NJ00464K>

12. 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) Volume 79, pages 2313–2335, (2025) <https://doi.org/10.1007/s11696-025-03927-7>
13. Abdellatif Rafik, Hafid Zouihri, Kinzy Charles, Kholood A. Dahlous, Mohammad Shahidul Islam, **Nivedita Acharjee**, Mohammed Salah & Abdellah Zeroual (2025) Novel hybrid material H7N2O4P: crystallographic and molecular analysis with insights into its anticancer potential, *Chemical papers (Springer)* (IF: 2.1) Volume 79, pages 941–959, (2025) <https://doi.org/10.1007/s11696-024-03828-1>

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15. 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>
16. 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>
17. 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)
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20. 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 nitron 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>
21. Jamelah S Al-Otaibi*, Y.Sheena Mary, Y.Shyma Mary, **Nivedita Acharjee**, Abdulaziz A. Al-Saadi, Maria Cristina Gamberini (2024) Influence of pyramidal M20 (M=Cu, Ag, Au) clusters on SERS

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