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Research Publications

30. D. Sarkar, N. Sehrawat, S. Yadav, S. Palatsingh, P. Lama, M. Gupta, R. K. Metre "Electrocatalytic Water Oxidation by a Heterogenized Co (III)–Aminophenol Complex: Structure–Activity Relationship and DFT Mechanistic Insight" *Chem. Asian J.* 2026 (Accepted)
29. S. Bhattacharyaa, M. Rahamana, S. Suman, D. K. Rout, S. Mondala, S. Purward, B. Dhingrae, P. C. Shuklaa, G. Mukherjee, M. Gupta, D. Guha, M. K. Bhattacharya, T. K. Dolai, N. Chakravorty, B. Mukherjee "HLA Polymorphisms Shape Divergent Outcomes of Toxoplasma and Plasmodium infection in Eastern Indian HbE/ β -Thalassemia Cohort " *Commun. Biol.* 2026 (Accepted)
28. S. Yadav, U. B. Yadav and M. Gupta "Hybrid polythiophene–metal composites as promising sensing materials for chemical warfare agents and chlorofluorocarbons" *RSC Adv.* 2026, 16, 11686 <https://doi.org/10.1039/D6RA00636A>
27. A. Joshi and M. Gupta* "Regulatory role of O₃ acetylation as a molecular switch in xylan-cellulose interactions." *Cellulose* 2026. <https://doi.org/10.1007/s10570-026-06960-1>
26. C S Keerthana, T. Kundu, M. Beura, S. Chakraborty, V. Verma, D. Kamil, M. Gupta*, V. Krishnan "Conformation-Driven Extraction Strategies for Lentinan: Integrating Sub-critical Water Extraction Techniques and Molecular Simulations for High-Value Functional Food Development Towards a Sustainable Bioeconomy" *Proc. Indian Natl. Sci. Acad.* 2025, 91, 1472 <https://doi.org/10.1007/s43538-025-00573-1>
25. S. F. Elahi, A. A. Khan, S. Yadav, M. Gupta, E. Ahmad "[A Facile Synthesis of Butyl Butyrate as a Sustainable Aviation Fuel via Sulfonated Graphene Oxide Catalysis](#)" *Top. Catal.* 2026, 69, 1029-1044 <https://doi.org/10.1007/s11244-025-02196-8>
24. S. Yadav, E. Ahmad, M. Gupta* "Computational Studies to Explore the Role of Ni-Decorated Nanocages Comprising p-block Elements for CO₂ Sequestration" *ChemistrySelect* 2025, 10, e02916 <https://doi.org/10.1002/slct.202502916>
23. A. Bi, S. Mahmood, N. Garg, S. Thakur, S. A. Chaudhry, S. Yadav, M. Gupta, M. Bechelany, J. Prakash, Z. Haque "Graphene oxide/polyindole nanocomposite: a highly efficient multi-cyclic, stable and sustainable photocatalyst platform for wastewater remediation under visible light" *Mater. Adv.* 2025, 6, 6320-6336 <https://doi.org/10.1039/D5MA00429B>

22. A. Joshi, Z. Xiao, S. Suman, C. Cooper, K. Ha, J. A. Carson, L. D. Quarles, J. C. Smith, M. Gupta* "Structure-Based Design of Small-Molecule Inhibitors of Human Interleukin-6" *Molecules*, 30, 2919 <https://doi.org/10.3390/molecules30142919>
21. S. F. Elahi, S. Prasad, M. A. Haider, M. Gupta*, E. Ahmad, "Congruity of Butyl Butyrate and Limonene as Potential Blends to Produce Green and Sustainable Aviation Fuels", *J. Chem. Eng. Data*, 2025, 70, 2713 <https://doi.org/10.1021/acs.jced.5c00131>
20. J. Kala, V. Dhonge, S. Ghosh, M. Gupta*, S. Basu, B. K. Mani and M. A. Haider "In silico design and experimental validation of a high-entropy perovskite oxide for SOFC cathodes" *J. Mater. Chem. A*, 2025, 13, 21916-21928 (Featured in Women's day collection of RSC Materials Portfolio) <https://doi.org/10.1039/D4TA08251F>
19. T. Kundu, J. Smith and M. Gupta* "Effect of Acetylation Patterns of Xylan on Interactions with Cellulose" *Biomacromolecules* 2025, 26, 1659 <https://pubs.acs.org/doi/10.1021/acs.biomac.4c01469>
18. M. Abbas, A. A. Septevani, F. Yurid, A. Joshi, M. Gupta, S. M. Rangappa, G. M. Madhu, M. Sriariyanun, S. Siengchin & P. Baranitharan "Thermal interface polymer-based composites materials: a critical review" *Multiscale and Multidiscip. Model. Exp. and Des.* 2025, 8, 191. <https://doi.org/10.1007/s41939-025-00787-2>
17. I. Raheem, A. Tawai, S. Amornraksa, M. Sriariyanun, A. Joshi, M. Gupta, W. Pongprayoon, D. Bhattacharyya and S. K. Maity "A Comprehensive Review of Approaches in Carbon Capture, and Utilization to Reduce Greenhouse Gases" *Appl. Sci. Eng. Prog.* 2025, 18, 7629 [dx.doi.org/10.14416/j.asep.2024.11.004](https://doi.org/10.14416/j.asep.2024.11.004)
16. A. Joshi, M. Gupta* and T. Phusantisampan "Harnessing Genetic Engineering for Enhancing Lignocellulose Biomass Production" *Appl. Sci. Eng. Prog.* (Editorial corner article) 2025, 18, 7614 [10.14416/j.asep.2024.09.013](https://doi.org/10.14416/j.asep.2024.09.013)
15. D. Jose, S. Vasudevan, P. Venkatachalam, S. Maity, A. Septevani, M. Gupta, P. Tantayotai, H. Bari, M. Sriariyanun "Effective deep eutectic solvent pretreatment in one-pot lignocellulose biorefinery for ethanol production" *Ind. Crop. Prod.* 2024, 222, 119626 <https://doi.org/10.1016/j.indcrop.2024.119626>
14. M. Gupta*, P. Dupree, J. C. Smith and L. Petridis "Patterns in interactions of variably acetylated xylans with hydrophobic cellulose surfaces" *Cellulose* 2023, 30, 11323 <https://doi.org/10.1007/s10570-023-05584-z>
13. P. Khatua, S. Mondal, M. Gupta and S. Bandyopadhyay "In Silico Studies to Predict the Role of Solvent in Guiding the Conformations of Intrinsically Disordered Peptides and Their Aggregated Protofilaments" *ACS Omega*, 2022, 7, 43337 <https://doi.org/10.1021/acsomega.2c06235>
12. P. Khatua, M. Gupta and S. Bandyopadhyay "Exploring Heterogeneous Dynamical Environment around an Ensemble of A β 42 Peptide Monomer Conformations" *J. Chem. Inf. Model* 2022, 62, 3453 <https://doi.org/10.1021/acs.jcim.2c00593>
11. Haseena K. V, M. Gupta*, A. Madhu, A. Narang, M. I. Alam and M. A. Haider "Understanding Catalyst Inhibition from Biogenic Impurities in Transfer Hydrogenation of a

Biorenewable Platform Chemical” *J. Environ. Chem. Eng.* 2022, 10, 107132 <https://doi.org/10.1016/j.jece.2022.107132>

10. S. Prasad and M. Gupta* "Solvation of gold nanoparticles passivated with functionalized alkylthiols: A molecular dynamics study" *J. Mol. Liq.* 2022, 347, 118342 <https://doi.org/10.1016/j.molliq.2021.118342>

9. M. Gupta, T. Rawal, P. Dupree, J. C. Smith and L. Petridis ‘Spontaneous Rearrangement of Acetylated Xylan on Hydrophilic Cellulose Surfaces’ *Cellulose*, 2021, 28, 3327 <https://doi.org/10.1007/s10570-021-03706-z>

8. M. Gupta, K. Ha, R. Agarwal, D. Quarles and J. C. Smith ‘Molecular Dynamics Analysis of The Binding of Human Interleukin-6 with Interleukin-6-alpha-Receptor’ *Proteins*, 2020, 89, 163 <https://doi.org/10.1002/prot.26002>

7. D. M. Close, C. Cooper, P. Chirania, X. Wang, M. Gupta, J. Ossyra, R. J. Giannone, N. Engle, T. Tschaplinski, J. C. Smith, L. Hedstrom, J. M. Parks and J. K. Michener ‘Horizontal transfer of a pathway for coumarate catabolism unexpectedly inhibits purine nucleotide biosynthesis’ *Mol. Microbiol.* 2019, 112, 1784 <https://doi.org/10.1111/mmi.14393>

6. M. Gupta, P. Khatua, C. Chakravarty and S. Bandyopadhyay ‘Hydration Behavior along the Folding Pathway for Trpzip4, Trpzip5 and Trpzip6’ *J. Phys. Chem. B*, 2018, 122, 1560 <https://doi.org/10.1021/acs.jpcb.7b10135>

5. M. Gupta, T. S. Khan, M. Agarwal and M. A. Haider ‘Understanding the Nature of Amino Acid Interaction with Pd (111) or Pd-Au Bimetallic Catalysts in the Aqueous Phase’ *Langmuir* 2018, 34, 1300 <https://doi.org/10.1021/acs.langmuir.7b03271>

4. M. Gupta, T. S. Khan, S. Gupta, Md. I. Alam, M. Agarwal and M. A. Haider ‘Non Bonding and Bonding Interactions of Biogenic Impurities with the Metal Catalyst and the Design of Bi-Metallic Alloys’ *J. Catal.* 2017, 352, 542 <https://doi.org/10.1016/j.jcat.2017.06.027>

3. M. Gupta, P. Khatua, C. Chakravarty and S. Bandyopadhyay ‘The Sensitivity of Folding Free Energy Landscapes of Trpzip to Mutations in the Hydrophobic Core’ *Phys. Chem. Chem. Phys.* 2017, 19, 22813 <https://doi.org/10.1039/C7CP03825A>

2. M. Gupta, C. Chakravarty and S. Bandyopadhyay 'Sensitivity of Protein Glass Transition to the Choice of Water Model' *J. Chem. Theory Comput.* 2016, 12, 5643 <https://doi.org/10.1021/acs.jctc.6b00825>

1. M. Gupta, D. Nayar, C. Chakravarty and S. Bandyopadhyay 'Comparison of hydration behavior and conformational preferences of the Trp-cage mini-protein in different rigid-body water models' *Phys. Chem. Chem. Phys.* 2016, 18, 32796 <https://doi.org/10.1039/C6CP04634G>

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Patents

1. Shariq Farhan Elahi, Khwaja Alamgir Ahmad, Afaq Ahmad Khan, Ejaz Ahmad, Sarita Yadav, Madhulika Gupta, “A Process for Butyl Butyrate Production Using a V2O5-Supported Silicomolybdic Acid Catalyst”. Indian Institute of Technology (ISM), Dhanbad, Application No. 202531044349 (Granted)

Themed collection

1. An article titled “Toward Simulation-Guided Chemistry: Integrating Computational and Experimental Approaches in India” published in a special issue on “Policies to catalyse India’s innovation ecosystem” on 27th February 2026 by the Royal Society of Chemistry authored by Madhulika Gupta and Ankit Joshi.

Book chapters

1. T. Kundu, S. Suyash, M. Gupta* and B. Chowdhury Chapter "Introduction to Greenhouse Gases Composition and Characteristics" in Advances and Technology Development in Greenhouse Gases Book Series Vol. 1, Elsevier, 2024
2. M. Gupta, T. S. Khan, M. Agarwal and M. A. Haider “Noncovalent Interactions of Biogenic Impurities with Ni (111) and Pd (111), Bimetallic Alloys and Segregated Surfaces”, Catalysis Series No. 36, Noncovalent Interactions in Catalysis, The Royal Society of Chemistry, 2019 <https://doi.org/10.1039/9781788016490>

Conference Proceedings

1. S. Bhattacharya, M. Rahaman, S. Suman, M. Gupta, B. Mukherjee, N. Chakravorty "Taming the trojan horse: unwinding the complex relationship between HLA alleles and Apicomplexan infection in HbE/ β -thalassaemic patients at Molecular Parasitology Meeting at Woods Hole, Massachusetts USA from September 15-19th 2024.
2. M. Gupta, T. S. Khan, S. Gupta, Md. I. Alam, M. Agarwal and M. A. Haider ‘(582h) Understanding Heterogeneous Catalyst Deactivation by Biogenic Impurities on Ni (111) Surface and Bimetallic Alloy’ at 2017 AIChE Annual Meeting, Minneapolis, MN, U.S.A.
3. M. Gupta, D. M. Close, C. Cooper, P. Chirania, X. Wang, J. Ossyra, R. J. Giannone, N. Engle, T. Tschaplinski, J. C. Smith, L. Hedstrom, J. M. Parks and J. K. Michener “Understanding the structural and dynamic changes that relieve inhibition of IMPDH upon horizontal transfer of a pathway for coumarate catabolism into E. coli” at Biophysical Society Annual Meeting 2020 at San Diego, California, U.S.A. from February 15-21, 2020. <https://doi.org/10.1016/j.bpj.2019.11.2781>