Dr. Madhulika Gupta
Assistant Professor,
Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM)
Dhanbad, India
E-mail: madhulikagupta@iitism.ac.in

Scientific Publications:

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**, S. Bandyopadhyay "Exploring Heterogeneous Dynamical Environment around an Ensemble of Aβ 42 Peptide Monomer Conformations" *J. Chem. Inf. Model* 2022, 62, 3453 **https://doi.org/10.1021/acs.jcim.2c00593**

11. H. K. V, **M. Gupta****, A. Madhu, A. Narang, Md. I. Alam, 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, 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 α-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, 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

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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 Trpzips 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

Book chapters:

2. 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, 2023 (Just accepted)

1. **M. Gupta**, T. S. Khan, M. Agarwal and M. A. Haider **"**Noncovalent Interactions of Biogenic Impurities with Transition Metal Catalyst Surfaces", Catalysis Series No. 36, Noncovalent Interactions in Catalysis, The Royal Society of Chemistry, 2019
https://doi.org/10.1039/9781788016490

Proceedings of Conference:

1. **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.

2. **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

Featured on the cover page:

M. Gupta, T. Rawal, P. Dupree, J. C. Smith, L. Petridis
'Spontaneous Rearrangement of Acetylated Xylan on Hydrophilic Cellulose Surfaces' *Cellulose* 2021, **28**, 3327-3345
https://doi.org/10.1007/s10570-021-03706-z