Dr. Madhulika Gupta

Assistant Professor
Department of Chemistry and Chemical Biology
Indian Institute of Technology (ISM) Dhanbad
Jharkhand, India-826004

CONTACT ME AT

Office Address: Room No. 101, Department of Chemistry and Chemical Biology, IIT (ISM) Dhanbad, Jharkhand - 826004,India

madhulikagupta@iitism.ac.in

https://people.iitism.ac.in/~madhulikagupta/

COMPUTATIONAL SKILLS

- TCL Scripting, VMD, MATLAB
- C, C++, FORTRAN, Python, CUDA
- GROMACS, NAMD, LAMMPS, DL_POLY, OPENMM
- ROSETTA, MOE, Autodock, Autodock Vina
- Gaussian, Materials Studio
- HPC Computing : HPC (IIT Delhi), TITAN (ORNL), SUMMIT (ORNL), NERSC (ORNL)

COURSES TAUGHT

- Introduction to Computational Chemistry
- Quantum Chemistry
- Computer aided drug discovery
- Research Methodology and Statistics
- Numerical Analysis and Methods in Chemistry
- Engineering Chemistry
- Introduction to Molecular Biophysics
- Protein Dynamics
- Physical Chemistry
- Environmental Chemistry

AWARDS RECEIVED

- Shailja Memorial Book Grant, University of Delhi
- Science Meritorious Award
- Summer Research Fellowship, Indian Academy of Sciences

CompCatCollab:
Computational Biophysics Lab is a part of CompCatCollab run by Renewable Energy Lab, Department of Chemical Engineering at IIT Delhi aimed at using homogeneous and heterogeneous catalysis for energy and environment applications.
More details available at:
https://www.reclab.in/compcatcollab

RESEARCH INTERESTS

Computational and Theoretical Chemistry :

- Understanding protein-protein interactions
- Computer aided drug discovery: high virtual throughput screening and ensemble docking, designing specific inhibitors for protein-receptor interactions
- Understanding the complex interplay of interactions between cellulose, hemicellulose and lignin in plant cell walls
- Assessing the relationships between sequence dependent specificity of peptides or amino acids (hydrophobic/ hydrophilic) as well as conformational preferences, hydration shell structural ordering and dynamics of peptides with different secondary structures
- Alternative design of bimetallic surfaces to curb the inimical effects of surface poisoning of catalyst surface by biogenic impurities

WORK EXPERIENCE

- **Assistant Professor**

- IIT(ISM) Dhanbad, Jharkhand, India | Present
- VIT Bhopal University, Bhopal, India | Sep 2020 - May 2021

- **Postdoctoral fellow**

-Oak Ridge National Lab, Oak Ridge, Tennessee, USA | May 2018 - Aug 2020
-Mentor for Appalachian Regional Commission/ Oak Ridge National Laboratory 2019 High School Summer Math Science Technology Institute | July 6-19, 2019

- **Assistant Professor**

St. Stephen's College, University of Delhi, Delhi, India | Aug 2017 - April 2018

EDUCATION

- **Ph.D. Computational Chemistry -** IIT Delhi, Delhi, India
- **M.Sc. Chemistry** (Specialization in Physical Chemistry)- St. Stephen's College, University of Delhi, Delhi, India
- **B.Sc. (HONS.) Chemistry** - St. Stephen's College, University of Delhi, Delhi, India

Research 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 -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 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 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

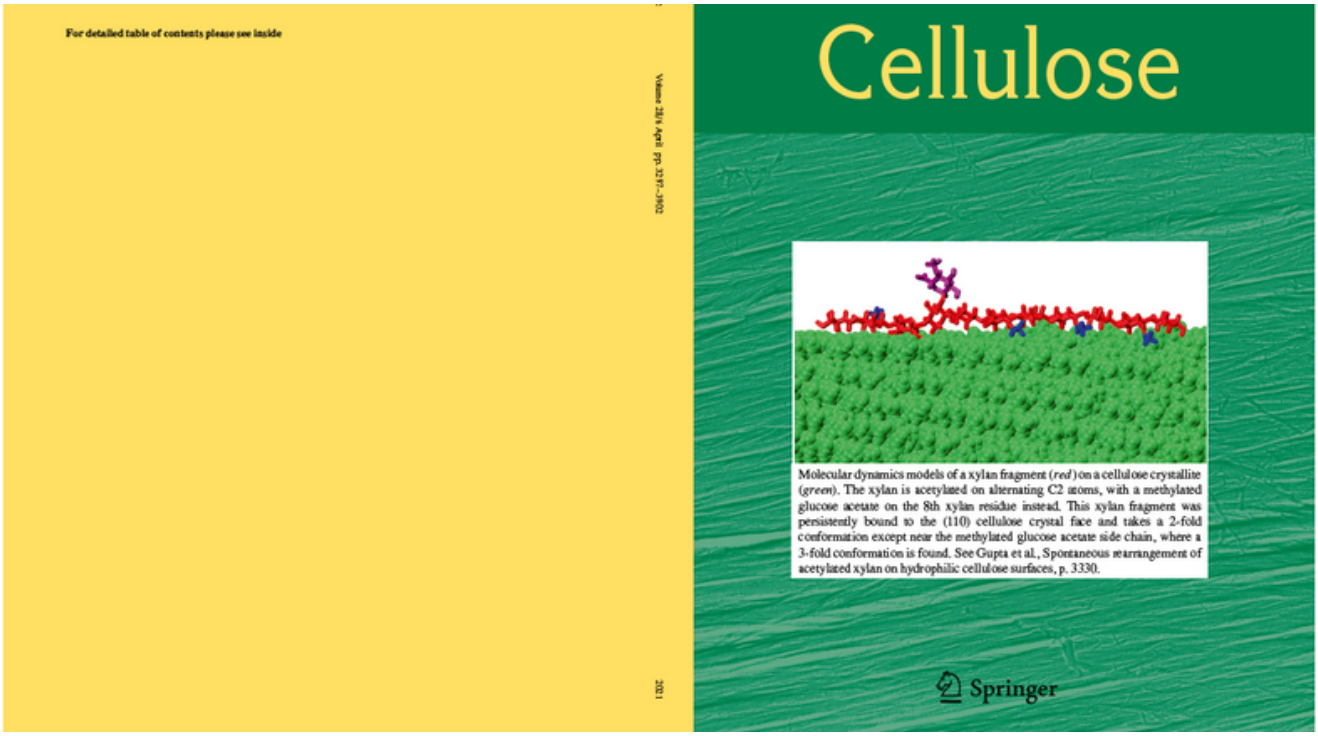
1. **M.Gupta**, D. Nayar, C. Chakravarty and S. Bandyopadhyay 'Comparison of hydration behavior and conformational preferences of the Trp-cage mini-protein in different rigid-body water models' Phys. Chem. Chem. Phys. 2016, 18, 32796 https://doi.org/10.1039/C6CP04634G

Conference Proceedings

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 https://doi.org/10.1007/s10570-021-03706-z



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 Ni (111) and Pd (111), Bimetallic Alloys and Segregated Surfaces" in Noncovalent Interactions in Catalysis, *RSC Advances*, 2019 https://doi.org/10.1039/9781788016490

International Oral Presentations

1. "Role of position and pattern of acetylation in xylan-cellulose interactions" at ACS Fall 2022 from August 21-25, 2022.
2. "Spontaneous change in O-2 acetylated xylan conformations on the (110) hydrophilic cellulose surface" at ACS Spring 2021 from April 5-30, 2021.
3. "Understanding heterogeneous catalyst deactivation by biogenic impurities" presented in "21st Annual Green Chemistry and Engineering Conference" held at Hyatt Regency, Reston, Virginia, U.S.A. from June 13-15, 2017.

Invited Talks

1. "Advances in Computational Chemistry" in Computational Chemistry Symposium 2023 at VIT Bhopal University on 2nd February 2023.
2. Motivating tribal school children to pursue research career in science, engineering and technology under the DST funded project on "Motivate School Students and Teachers Concerning the relevance of Science and Technology through Innovative Communication Techniques" on 11th December 2022.
3. "Understanding Biomolecular Recognition in Human Interleukin for Therapeutic Intervention" in 27th ISCB International Conference (ISCBC-2022) entitled "Research and Innovation in Chemical, Pharmaceutical, and Biological Sciences" at BIT-Mesra Ranchi, Jharkhand, India on 18th November 2022.
4. Talk on "Molecular Dynamics Simulations: Hands-On" in Refresher course in Chemistry on Emerging Trends in Chemical Sciences by UGC- Human Resource Development Centre, Ranchi University, Jharkhand, India on 25th August 2021.
5. Talk on "Introduction to Computational Chemistry" in Refresher course in Chemistry on Emerging Trends in Chemical Sciences by UGC- Human Resource Development Centre, Ranchi University, Jharkhand, India on 19th August 2021.

Grants Received as Sole PI

3. SERB POWER Grant of INR 28,25,900/- for project titled "Deconstruction of Lignocellulosic Biomass for Bioenergy" by DST (SERB) [Department of Science and Technology (Science and Engineering Research Board)]| July 2022 - 2025

2. Grant of INR 11,00,000/- for project entitled "Understanding Bio-molecular Recognition in Human Interleukin-6 (hIL-6) Complex and Designing Antagonists for hIL-6" by IIT(ISM) Dhanbad | December 2021 to Present

1.Grant of INR 25,25000/- for project entitled "Free energy landscape for Trpzipper4, Trpzipper5 and Trpzipper 6" by High Performance Computing (HPC), IIT Delhi | Sep 2016 to Mar 2017

Grants Received as co-PI

Grant of INR 4,50,000/- for 2 days national workshop on "Low-Cost Bio-coal Production and Its Potential Impact on Steel Industries" by DSIR (Department of Scientific and Industrial Research)| May 14-15, 2022.

Conferences/workshops organized

1. Joint Secretary in core committee for organizing an international conference on "Recent Trends Chemical Sciences-2022 (RTCS-2022)" hosted by Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad under the aegis of Indian Chemical Society from 16-18th December.

2. Co-organizing secretary for organizing a DSIR supported two days national workshop on “Low-Cost Bio-coal Production and Its Potential Impact on Steel Industries” at IIT (ISM) Dhanbad from 14th-15th May 2022.
3. Member of the organizing committee for 2nd National Conference on “Recent Trends in Applied Sciences and Computing Engineering” held at VIT Bhopal University from 18-20th December 2020.
4. Coordinating and organizing National Conference on "Chemical Sciences: Opportunities and Challenges 2018” held at St. Stephen’s College, Delhi, India from March 19-20, 2018.
5. Volunteer for organizing Indo-US Bilateral workshop on “Nanoparticle Assembly: From Fundamentals to Applications” held at IIT Delhi, Delhi, India from December 12-14, 2011.

Administrative Responsibilities

1. Member of Fete and Cultural, Food and Catering committee for BASANT-2023 & III-2023 scheduled to be held on 4th & 5th February 2023 at IIT(ISM) Dhanbad.
2. Supervision for smooth execution and deliberation of pre-convocation and convocation food during 41st convocation 2022.
3. Warden for Girl's hostel (Rosaline and Ruby Hostel) at IIT (ISM) Dhanbad from July 2022 to Present.
4. Departmental Faculty coordinator for International Relations at IIT (ISM) Dhanbad from 2021 to present.
5. Member of the beautification committee of the Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad.

Additional Responsibilities

1. Invited Jury member for 30th District Level National Children's Science Congress 2022 & 25th District Level Child Rights' Congress 2022 on the theme "Understanding Ecosystem for Health and Well-Being" on 3rd December 2022.
2. Invited session chair for "National Conference on Molecular Modeling and Simulations" (NCMMS 2022) held at VIT Bhopal University from February 28 to March 02, 2022.

Thesis supervision

a) Ph.D.

3. Mithu Kumari (2022) - JRF
2. Praveen Kumar (2022) joint Ph.D. student from IIT Delhi
1. Tripti Kundu (2021) - PMRF Fellow

b) M.Tech in Pharmaceutical Science and Engineering:

4. Ms. Shreya Suman (2022-2024)
3. Mr. Pritam Singh (2022-2024)
2. Mr. Shreyansh Suyash (2021-2023)
1. Ms. Rajeshwary Shil (2021-2023)

c) M.Sc. Chemistry

6. Deepak Kumar Meena (2021-2023)
5. Naina Karmakar (2021-2023)
4. Chandan Majhi (2021-2023)
3. Anisha Pegu (2020-2022)
2. Shubham Mudi (2020-2022)
1. Nitish Barik (2020-2022)

Conferences/ Workshops/ Symposia:

1. Attended 26th International Symposium on Chemical Engineering (ISCRE 26) and the 9th Asia-Pacific Chemical Engineering (APCRE 9) Symposium held at IIT Delhi from December 5-8, 2021.
2. Attended CHARMM-GUI CECAM School from September 5-10, 2021.
3. Webinar on "Targeted Delivery of RNA-targeted Therapeutics" by ACS on July 29, 2021.
4. Poster presentation titled “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.
5. Attended CADES NVIDIA GPU BASICS workshop in Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. on November 11, 2019.
6. Participated in “National Conference on Scientific Innovation-A Head Start” held at St. Stephen’s College, Delhi, India from April 5-6, 2018.
7. Participated in “National Conference on Chemical Sciences: Opportunities and Challenges 2018” held at St. Stephen’s College, Delhi, India from March 19-20, 2018
8. Presented poster titled “Comparison of Hydration Behaviour and Conformational Preferences of Trp-cage Mini-protein in Different Rigid Body Water Models” in “Nanoparticle Assembly - From Fundamental to Applications : Faraday Discussions” held at IIT Bombay, Mumbai, Maharashtra, India from January 7-9, 2016.
9. Presented poster titled “Sensitivity of Local Hydration Behaviour and Conformational Preferences of Peptide to the Choice of Water Model” in “Theoretical Chemistry Symposium 2014” held at NCL Pune, Pune, Maharashtra, India from December 16-18, 2014.
10. Presented poster titled “Sensitivity of Local Hydration Behaviour and Conformational Preferences of Peptide to the Choice of Water Model” in “The 3 M's of Chemistry : Molecules, Materials & Medicine” held at IIT Delhi, Delhi, India on December 11, 2014.
11. Presented poster titled “Sensitivity of Local Hydration Behaviour and Conformational Preferences of Peptide to the Choice of Water Model” in “Dynamics of Complex and Biological Systems (DCCBS14)”held at IIT Kanpur, Kanpur, India from February 13-15, 2014.
12. Satellite workshop on “Advances in Molecular Dynamics of Biomolecular Simulations” held at SC&IS, Jawaharlal Nehru University, Delhi, India from December 3-4, 2013.
13. Presented poster titled “Sensitivity of Local Hydration Behaviour and Conformational Preferences of Beta-sheet and Alpha-helical Peptides to Choice of Water Model” in “In-House Symposium:New Horizons in Chemistry” held at IIT Delhi, Delhi, India on November 16, 2013.
14. Presented poster titled “Molecular Dynamics Simulations of Trp-cage using CHARMM force field” in “Symposium on Biomolecules in Motion: Theory and Simulations” held at Jawaharlal Nehru University, Delhi, India from January 4-6, 2013.
15. Presented poster titled “Molecular Dynamics Simulations of Trp-cage using CHARMM force field” in “Theoretical Chemistry Symposium 2012” held at IIT Guwahati, Guwahati, Assam, India from Decembe 19-22, 2012.
16. Presented poster titled “Molecular Dynamics Simulations of Trp-cage using CHARMM force field” in “New Directions in Chemical Sciences” held at IIT Delhi, Delhi, India from December 7-9, 2012.
17. Presented poster titled “Molecular Dynamics Simulations of Trp-cage using CHARMM force field” in “International Symposium on Protein folding and dynamics” held at National Centre for Biological Sciences (NCBS), Bangalore, India from October 15-17, 2012.
18. Attended Indo-US Bilateral workshop on “Nanoparticle Assembly: From Fundamentals to Applications” held at IIT Delhi, Delhi, India from December 12-14, 2011.

19. Attended “Chemistry- Structure, Reaction Dynamics and Spectroscopy” held at St. Stephen's College, University of Delhi, Delhi, India from August 21-23, 2008.