

CURRICULUM VITAE



Name : Lt (Dr.) *MADHULATA SHUKLA*

DOB : 28th December 1984

Designation : Assistant Professor (Senior) & HEAD

Present Address : Department of Chemistry
G. B. College, Ramgarh
Kaimur, 821110
Veer Kunwar Singh University
Bihar

E-mail : madhu1.shukla@gmail.com,
madhulata.pf.chy17@itbhu.ac.in

Webpage : <https://madhulatashukla.wixsite.com/mls-lab>

Important IDs:

Orcid Id :- 0000-0002-4060-8729
Scopus Id :- 36159888200
Researcher Id :- AAG-2940-2020
Google Scholar Id :- AVOjS_gAAAAJ
Vidwan Id :- 146790

Education:

- Ph.D, 2014, Banaras Hindu University [Ph. D. Thesis Title: *Spectroscopic and DFT studies of Ionic Liquids, Donor –Acceptor Organic molecules and Inorganic complexes.*]; Supervisor Name: Dr. Satyen Saha
- M.Sc., 2008, Banaras Hindu University

Experience:

- **National Post-Doctoral Fellow, SERB** from Indian Institute of Technology (Banaras Hindu University) 11th July 2017 - 31st Oct. 2017.
- Assistant Professor (1st Nov. 2017 - 31st Oct. 2021)
- Senior Assistant Professor & Head (1st Nov 2021 - till date)

Membership of Professional Bodies:

- Life Member: Indian Science Congress Association (ISCA)
- Life Member: Chemical Research Society of India (CRSI)
- Life Member: Society for Material Chemistry (SMC)
- Convener of Chemical Research Society of India, Bihar & Jharkhand Chapter (2023-2027)
- Editorial board member of International Journal of Computational & Theoretical Chemistry (2018-21)
- Editor of Frontiers in Nanotechnology Journal (2023-24)
- Guest Editor of International Journal of Photochemistry and Photochemical Research <https://journals.stmjournals.com/editor-detail/profile/209153/>

Awards:

- Received **Major UGC Start-up grant Project** (Title: Molecular Mechanism and Catalytic Study for the Activation of Ag/Cu nanoclusters and their bimetallic by imidazolium based Ionic Liquids.) in 2018 (Rs. 10 Lakhs) and completed successfully.
- Worked as Poster Presentation judge at July, CRSI 2022 conference held at IISER Mohali and July, CRSI 2023 conference held at NIT Rourkela.
- Best Poster presentation Award from Chemical Research Society of India in CRSI 2013 symposium.
- Qualified Graduate Aptitude Test in Engineering (GATE, Chemistry, 2010) **AIR-94**.
- Qualified National Eligibility Test (NET) (UGC-**JRF**, June, 2010)

Research Interest:

- Spectroscopy, DFT calculation,
- Ionic Liquids, Nanoparticles
- Donor-Acceptor molecules

List of Publications:

- [1]Bronsted acidic surfactant [HDMM]⁺ [HSO₄]⁻: A Green microreactor assembly for stereoselective synthesis of novel thiazolyl-pyrazole-chromen-2-ones in water Patil, M.; Mhaldar, P.; Mahadik, V.; Ghanta, R.; Shukla, M.; Sonawane, S.; Ghotekar, S.; Rashinkar, G.; Pore, D. *RSC Advances* **2025**, 15, 13753 .
- [2]Curcumin-mediated synthesis of cuprous oxide nanoparticles and its photocatalytic application R. Ranjan, M. Shukla* *Next Materials*, **2025**, 6, 100481. <https://doi.org/10.1016/j.nxmte.2024.100481>.
- [3]Synthesis of copper (II) oxide nanoparticle: A promising material for photocatalysis R. Ranjan, M. Shukla* *Materials Protections* 66 (2025) <https://doi.org/10.62638/ZasMat1227>
- [4]Synthesis of Magnetically Recoverable Nickel (II) Complex-Functionalized Fe₃O₄@ISNA (ISNA= Isonicotinic Acid) Nanomaterials: Catalytic Studies on Nitrophenol Reduction and TD-DFT studies R. Mondal, R. Ghanta, M. Shukla, T. Chattopadhyay *Journal of Polymer & Composites* **2024**, 13, 88-96.
- [5]Synthesis of Copper(II) Complex-functionalized Fe₃O₄@ISNA (ISNA=Isonicotinic acid) as magnetically recoverable nanomaterials: catalytic studies on Alcohol oxidation, Nitrophenol reduction and TD-DFT studies. R. Mondal, A. Chakraborty, M. Shukla* and T. Chattopadhyay* *New J. Chemistry*, **2024**, **48**, 7308-7322. <https://doi.org/10.1039/D3NJ05440C>
- [6]Molecular Interaction of Curcumin with Silver Nanocluster: A DFT Study D. Gupta, R. Ranjan, and M. Shukla* *Vib. Spectr.* 129, **2023**, 103604.
- [7]Green synthesis of silver nano-catalyst using ionic liquid and their photocatalytic application to the reduction of *p*-nitrophenol R. Ranjan, D. Gupta, and M. Shukla* *Eur. J. Chem.* 14 (3) **2023**, 316.
- [8]Imidazole-Based Bronsted Acidic Surfactant: A Novel Regioselective Catalytic System for Making of 2-Aryl-1,2-Dihydrothiazolo[3,2-b][1, 2, 4]Triazol-6(5*H*)-Ones M. V Patil, P. M Mhaldar, M. Shukla, A. N Srivastva, D. M. Pore *Polycyclic Aromatic Compounds* **2022**, 1-18. doi.org/10.1080/10406638.2022.2118327

- [9] Ionic Liquid Functionalized Cu₂O nanoparticles **Shukla M.***, Pal S., Sinha I. *J. Mol. Struct.* **2022**, 1262, 132961. doi.org/10.1016/j.molstruc.2022.132961.
- [10] Experimental and DFT Calculation Study of Interaction between Silver Nanoparticle and 1-butyl-3-methyl Imidazolium tetrafluoroborate Ionic Liquid; **Shukla M.***, verma A. D., Kumar S., Pal S., Sinha I. *Heliyon* ,7, **2021**, e6065.
- [11] Mechanism of visible light enhanced catalysis over curcumin functionalized Ag nanocatalysts Verma A., **Shukla M.**, Kumar S., Pal S., Sinha I., *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2020**, <https://doi.org/10.1016/j.saa.2020.118534>.
- [12] Experimentally formulated and theoretically rationalized alumina immobilized copper catalyst for alcohol oxidation Chowdhury T., Chatterjee S., Banerjee P., Sukul D., **Shukla M.***, Chattopadhyay T, J. *Coordination Chemistry*, **2020**, 73, 754-771.
- [13] Ag-Cu bimetallic nanoparticles as efficient oxygen reduction reaction electrocatalysts in alkaline media, Verma A., Gupta R., **Shukla M.**, Malviya M., Sinha I., *Journal of Nanoscience and Nanotechnology* 20, **2020**,1765–1772.
- [14] Adsorption mechanism of phenol, p-chlorophenol, and p-nitrophenol on magnetite surface: A molecular dynamics study Kuntail J., Yash. R., **Shukla M.**, Sinha I. *J. Molecular Liquids* **2019**, 1110531.
- [15] ZnO–Bentonite nanocomposite: an efficient catalyst for discharge of dyes, phenol and Cr(VI) from water Chakraborty T. , Chakraborty A., **Shukla M.***, Chattopadhyay T.* *Journal of Coordination Chemistry* **2019** doi.org/10.1080/00958972.2018.1560429. (Cover Page)
- [16] Syntheses and characterization of mononuclear Zn(II), Cd(II) and Hg(II) complexes of 2-[(3,5-Dibromo-2-hydroxy-benzylidene)-amino] 2-hydroxymethyl-propane-1,3-diol: Photoluminescence properties and DFT study. Chatterjee, S.; Majumder, I.; Chakraborty, A; **Shukla, M.***; Chattopadhyay, T.* *Inorg. Chim. Acta* 2018, 471, 159-167.

- [17] *Catalytic activation of nitrobenzene on PVP passivated silver cluster: A DFT investigation.* **Shukla, M.**; Sinha I. *Int. J. Quantum Chem.* 2018; 118, e25490. doi.org/10.1002/qua.25490.
- [18] *Spectroscopic and DFT Studies of Cation-Anion Interaction in Imidazolium and Piperidinium Based Ionic Liquids* **Shukla, M.** 2017 *J. Scientific and Technical Research* Volume 3, Issue 1, June 2018. (Conference Proceeding)
- [19] *Hydrogen bonding interactions in nicotinamide Ionic Liquids: A comparative spectroscopic and DFT studies* **Shukla, M.*** *J. Mol. Struct.* 2017, 1131 275-280.
- [20] *Raman spectroscopic study of water tetramer in [Cu(3-aminomethyl) pyridine OH2oxalate-2H2O]_n,* **M. Shukla***, 2016, 105, 200-204. *Polyhedron*
- [21] *Ferrocenyl-cymantrenyl hetero-bimetallic chalcones: Synthesis, structure and biological properties.* Mishra, S.; Tirkey, V.; Ghosh, A.; Dash, H. R.; Das, S.; **Shukla, M.**; Saha, S.; Mobin, S. M.; Chatterjee S. *J. Mol. Struct.* 2015, 1085, 162–172.
- [22] *Importance of weak interactions and conformational equilibrium in N-butyl-N-methylpiperidiniumbis(trifluoromethanesulfonyl) imide room temperature ionic liquids: Vibrational and theoretical studies.* **Shukla, M.**; Noothalpati, H.; Shigeto, S.; Saha, S. *Vib. Spect.* 2014, 75, 107-117.
- [23] *Solvent induced geometry transformation of trigonal planar Cu(I) complexes of N-((2/4-methoxy carbonyl) phenyl)-N0-(ethoxy/methoxycarbonyl) thiocarbamides to square-planar Cu(II) complexes: Synthesis, spectral, single crystal, DFT and in vitro cytotoxic study:* Singh, D. P.; Pratap, S.; **Shukla, M.** *Inorg. Chim. Acta* 2014, 423, 386-396.
- [24] *Influence of Metal to Ligand Molar Ratios on the Supramolecular Structure Formation of Cu(II) with diaminopropane and Iodide: Synthesis, Structure, Spectroscopic and DFT Studies:* Kharedia, B.; **Shukla, M.**; Saha, S.; Sunkari, S. *J. Mol. Struct.* 2014, 1062, 158-166.
- [25] *Synthesis of mono- and bi-metallic dithiocarboxylate-alkyne complexes from sunlight driven insertion reaction and their antibacterial activity:* Patel, S. K.; Tirkey, V.; Mishra, S.; Dash, H. R.; Das, S.; **Shukla, M.**; Saha, S.; Mobin, S. M.; Chatterjee, S. *J. Organomet. Chem.* 2014, 749, 75-82.

- [26] *Relationship between stabilization energy and thermophysical properties of different imidazolium ionic liquids: DFT studies.* Shukla, M.; Saha, S. **Comput. and Theor. Chem.** 2013, 1015, 27-33.
- [27] *Water Square (uudd) in Novel Cu^{II} Framework Structures Built from Isomeric (Aminomethyl)pyridines and Oxalate: Synthesis, Structure, Spectral and DFT studies.* Shukla, M.; Kharedia, B.; Srivastava, N.; Saha, S.; Sunkari, S.; **Polyhedron** 2013, 54, 164-172.
- [28] *Investigation of Ground State Charge Transfer Complex between Paracetamol and p-Chloranil through DFT and UV-visible studies.* Shukla, M.; Srivastava N.; Saha S. **J. Mol. Struct.** 2012, 1021, 153-157.
- [29] *An unusual way to synthesize 1-nitronaphthalene from 1-amino-5-nitronaphthalene* Srivastava, N.; Shukla M.; Saha S. **African J. Phar. Pharma.**, 2011, 5, 542-546.
- [30] *Synthesis, structure, UV-visible-IR spectra, magnetism and theoretical studies on Cu^{II}[(2-aminomethyl) pyridine] (thiocyanate)₂ and comparisons with an analogous Cu complex.* Shukla, M.; Srivastava, N.; Saha, S.; Rao T. R.; Sunkari, S. **Polyhedron** 2011, 30, 754-763.
- [31] *An unusual effect of charcoal on purification of alkylimidazolium iodide RTILs,* Srivastava, N.; Shukla M.; Saha S. **Ind. J. Chem.** 2010, 49A, 757-761.
- [32] *Theoretical and spectroscopic studied of 1-butyl-3-methylimidazolium iodide RTILs: Its differences with chloride and bromide derivatives.* Shukla M.; Srivastava N.; S. Saha **J. Mol. Struct.** 2010, 975, 349-356.

Book Chapters:

- [1] Molecular Self-Assemblies for scalable and tuneable applications in the efficient drug delivery, R. Dubey, S. Kumar, M. Shukla, in Molecular Self-Assemblies: Advanced Materials for Environmental and Sensing Applications, vol 1, 2024, pg 285 CRC Press, Taylor & Francis Group,

- [2] Metal- MXenes Interaction: Adsorption, Bonding, and Role of delocalized chemical bonding in “MXenes as Surface-Active Advanced Materials: book Madhulata Shukla, Sumit Kumar and Vikash Kumar, Elsevier Publication 2024. <https://doi.org/10.1016/B978-0-443-13589-7.00014-6>. ISBN: 978-0-443-13589-7
- [3] Ultrasound Irradiation: Fundamental Theory, Electromagnetic Spectrum, Important Properties, and Physical Principles Sumit Kumar, Amrural Prajapat, Sumit Kumar Panja, Madhulata Shukla in book entitled "Green Chemical Synthesis with Microwaves and Ultrasound" (WILEY-VCH publication) 2024 e Book ISBN: 978-3-527-35297-5
- [4] Synergism in Anticorrosive Phenomenon of Phytochemicals/ Plant Extracts in Phytochemistry in Corrosion Science: Plant Extracts and Phytochemicals as Corrosion Inhibitors M. Shukla Taylor & Francis (CRC Publication), 2024 eBook ISBN: 9781032496153
- [5] Variation of structural features and interactions with substitution of different alkyl for Imidazolium based ILs R. Ranjan, M. Shukla in book titled “Futuristic Trends in Chemical, Material Sciences & Nano Technology Volume 3, Book 24, Part 1, Chapter 1, pg 1-15 **2024**, Iterative International Publisher e-ISBN: 978-93-5747-617-1.
- [6] Carbon Allotropes in Corrosion Prevention: Computational-based Advancements M. Shukla & S. Kumar Taylor & Francis (CRC Publication), 2023 eBook ISBN: 9781003323976.
- [7] Effect of Ionic Liquids in Nanoparticle Synthesis: Interaction and Organization M. Kumari, D. Gupta & M. Shukla in book titled “Futuristic Trends in Chemical, Material Sciences & Nano Technology Volume 2, Book 12, Chapter 13, **2022**, Iterative International Publisher, ISBN: 978-93-95632-66-9
- [8] Introductory Chapter: Salient features of Nanocatalysis A.D. Verma, M. Shukla, I. Sinha edited by I. Sinha & M. Shukla InTech Publication, **2019** ISBN 978-1-78984-160-2.
- [9] *Catalytic activation of PVP-stabilized Gold/Silver cluster on p-Nitrophenol Reduction: A DFT Investigation*; Shukla M., Sinha I. book chapter in *DFT Calculations*, InTech Publication, **2017** ISBN 978-953-51-5682-6.

- [10] *A comparative study of Piperidinium and Imidazolium based Ionic Liquids: Thermal, Spectroscopic and Theoretical Studies* Shukla, M.; Saha, S. book chapter in ***Ionic Liquids - New Aspects for the Future***" edited by Jun-ichi Kadokawa, InTech Publication, **2013**, pp61-84 ISBN 980-953-307-626-8.
- [11] *Interaction and transitions in imidazolium cation based Ionic Liquids*, Shukla, M.; Srivastava N.; Saha, S. book chapter in ***Ionic Liquids - Classes and Properties***, edited by Scott T Handy InTech Publication, **2011**, pp 153-170, ISBN- 978-953-307-634-8.

Book Edited:

1. "Futuristic Trends in Chemical, Material Sciences & Nano Technology Volume 3, Book 12, **2024**, IIP Proceedings, 978-93-5747-617-1.
2. "Futuristic Trends in Chemical, Material Sciences & Nano Technology Volume 2, Book 12, **2022**, IIP Proceedings, ISBN: 978-93-95632-66-9.
3. "***Nanocatalysts***" Sinha I. (Editor), Shukla M. (Co-editor), InTech Publication, **2019**, 978-1-78984-160-2.

Invited Lectures in Seminar/conference/symposium (From 2018):

1. Invited Talk (Investigation of Molecular Interactions of Curcumin and Silver/Copper Nanoparticles through experimental and DFT Analysis) in International Conference **INNOST NANO – 2025** organized by the Department of Chemistry SGT University, Haryana held from 12th-14th Nov 2025.
2. Invited Talk (Synthesis of Copper (II) Oxide Nanoparticles using Curcumin and Investigation of Molecular Interactions through DFT Analysis) in International Conference **SoPhyC-2025** organized by the Department of Chemistry IIT Patna, Bihar held from 11th-14th Oct. 2025.
3. Invited Talk (Synthesis of Silver and Copper Oxide Nanoparticles using curcumin and its Photocatalytic Application) in International Conference on Chemistry of Materials for Sustainable Future (ICMS 2025) organized by the Department of Chemistry L.N

Mithila University, Darbhanga, Bihar held from 20th-21st March 2025.

4. Invited Talk (Curcumin-Mediated Synthesis of Silver and Copper Oxide Nanoparticles and Molecular Interaction Study Using DFT Calculation) in International Conference on Sustainable and Innovative Materials for Modern Life (ICSMML-2024) organized by the Department of Chemistry, Siddharth University, Kapilvastu, Uttar Pradesh held from 12-13th March 2024.
5. Invited Talk (Synthesis of Nanoparticles in Ionic Liquid and Photocatalytic Study Using Spectroscopic & DFT Techniques) and Session chaired in 2nd International Conference on Recent Trends in Materials Science & Devices organized by the Research Plateau Publishers and G. A. V Degree College, Patauda, Jhajjar, Haryana held from 29-31st December 2023.
6. Invited Talk in International Conference on Recent Trends in Materials Science & Devices organized by the Research Plateau Publishers and G. A. V Degree College, Patauda, Jhajjar, Haryana held from 22-23 July 2023.
7. Invited Talk (Green synthesis of Silver and Copper nanocatalysts using ionic liquid and their photocatalytic application to the reduction of p-nitrophenol) in International conference on Frontiers at the Chemistry- Allied Sciences Interface (FCASI-2023) organized by the Department of Chemistry held at the University of Rajasthan from 20th – 21st April 2023.
8. Invited Talk in National Conference on Materials and Devices (NCMD) (webinar) on “Ionic Liquids: A superior Solvent for Synthesis and Stabilization of Metal nanoparticles” held on 18 - 19 December-2020 organized by Department of Physics, Teerthanker Mahaveer University, Moradabad.
9. Invited Talk in International Conference (webinar) on "Strategy of self dependency in COVID 19 and application of some exotic materials in the field of Physics, Chemistry, Biology, Medicine and Engineering", Organized by S.V.P. College, Bhabua, VKS University and STAMI group held during 29th May to 31st May 2020.
10. Invited Talk in International Conference on Electron Microscopy & Allied Analytical Techniques (EMAAT-2019) organized by Department of Physics, HP University, Shimla “Importance of Weak interaction in Ionic Liquids” held during 7th June

2019 to 9th June 2019.

11. Invited Talk in 2nd International conference on "Energy, Functional Materials and Nanotechnology (ICEFN-2019)" & "Sustainable Environment Management (SEM-2019) organised by Department of Chemistry, D.S.B. Campus, Kumaun University, Nainital on "Cation-anion interaction study in different Imidazolium and Piperidinium based Ionic Liquids" held during 24th May to 26th May 2019.

12. Special Invited Lecture in Prof. Iqubal Bahadur Singh Memorial Lecture series on "Significance of Green Chemistry for Society & PG Students" held at Department of Chemistry, Veer Kunwar Singh University, Ara on 31st Jan 2019.

13. Invited Talk in International conference on Frontiers at the Chemistry- Allied Sciences Interface (FCASI-2023) organised by Department of Chemistry held at University of Rajasthan during 21st – 22nd Dec. 2018.

14. Invited Talk in National conference on Materials and Devices organised by Department of Physics, Sharda University, Noida held during 31st July 2018 to 1st Aug. 2018.

15. Two-day workshop on Lab Activities of School Science Teachers of Bihar organised by Jawahar Navodaya Vidyalaya, Kaimur held during 14th July 2018 to 15th July 2018.

16. Invited Talk in International Seminar on Green Chemistry: Synthesis, Processing and Devices (ISGCSPD-2018) organised by Department of Chemistry, Veer Kunwar Singh University, Ara held during 6th April 2018- 7th April 2018.

Organization of Conference/Workshop/Faculty Development Program

1. **Convener**, One-day Lecture Workshop on *Current Trends in Science & Technology: Rural Development* in collaboration with the Chemical Research Society of India (CRSI) on 29th March 2025.
2. **Convener**, Two days International Conference on Composite Materials for Environment Protection and Remediation (ICCMEPR- 2024) in collaboration with Research Plateau Publisher, Haryana, 2-3 July 2024.
3. **Organizing Secretary** Indian National Science Academy (INSA) Remote Lecture on topic "Adaptation of Extremophilic Organisms: The Survival Strategies" on 15th Sept. 2023

4. **Convener**, One-day Lecture Workshop on *Chemistry and our Society* in collaboration with the Chemical Research Society of India (CRSI) on 8th April 2023.
5. **Convener**, *Two Week Faculty Development Program on Libre Office Writer* organized in collaboration with Spoken Tutorial, IIT Bombay, 20th April to 3rd May 2020.
6. **Convener**, *National Seminar on Environmental Pollution & Remediation* (NSEPR 2018) (sponsored by EESL company), 1st Nov. 2018.

Ph.D Supervision

1. **Durga Gupta (2021-25)**
2. **Ravi Ranjan (2022-ongoing)**
3. **Manish Kumar (2025-ongoing)**