Curriculum Vitae

Personal Information

Name: Dr. Sarvesh K. Pandey

Date of birth: Jan 9, 1988

Email: sarvesh@manit.ac.in ; skpchmiitk@gmail.com

Contact No: +91 - 639 392 0557

Website (Profile): https://www.manit.ac.in/content/dr-sarvesh-k-pandey

https://sites.google.com/view/dskp-chm-esc

Current Position: Assistant Professor

Organization - Department of Chemistry, National Institute of Technology (**NIT**) Bhopal, Madhya Pradesh, India

Address for Communication- Dr. Sarvesh K. Pandey, Assistant Professor, Department of Chemistry, Maulana Azad - National Institute of Technology (**NIT**) Bhopal, Bhopal - 462 003, Madhya Pradesh (**India**)

Subject – Chemistry (Physical and Materials Chemistry)

Specialization

- Computational Chemical and Materials Science
- Systematic Parameterization of Multidimensional Variables Correlated with Experimental Insights
- Computational Astrochemistry

Current Area of Research Interest

Computational Chemical and Materials Science

- Computational Design and Characterization of Novel (Inorganic and Organic Species like Superhalogens, Superbases, Superacids, Supersalts, *etc.*) Molecules/Materials and Their Potential Applications.
- Smart Design and Wide-range Characterization of Smart Biocomposites based on Hydrogels (like PAM), Ceramics (like HAP), *etc.* (Prediction for experimental processing and its validation) and Interfacial Chemistry/Interaction Involved Therein.
- Understanding and Uncovering Features of Confinement Effects of Newly Designed Small Complexes Associated with Carbonaceous Materials (Quantum Dots, CNT, Graphene, Fullerene, Diamond, Their Prototypes, *etc.*) using the Molecular Surgery Approach.

- MM/QM and MD Simulations on Various Moderate to Large Chemical Systems.

AI/ML Driven Computational Chemical and Materials Science Experiments

- AI/ML-driven intelligence to enhance computational chemistry by enabling rapid property prediction, intelligent molecular and materials design, data-enabled simulations, automated reaction pathway analysis, and optimized computational workflows.

Computational Astrochemistry

- Understanding and Unravelling the Formation of Diverse Chemical and Biological (for life survival) Molecules (more than 300 interstellar molecules are reported) by Possible Formation Pathways through Concerted (Single Step)/Intermediate (Multistep) Molecular Reaction Mechanisms in the Interstellar Medium (ISM).
- Structural, Stability/Energetic, and Electronic Feature Analysis of Detected Chemical/Biochemical Species (including not detected yet or reported).

Fundamental Chemistry

- Understanding a Long-standing Problem of the Concept of Bond Path (not a well-understood concept, hitherto).
- Physical Interpretation of the Concept of Cis- and Gauche-Effect and their Quantification using the QTAIM, NCI-plot, RFC, IC/CC Parameters.
- Quantification of Aromaticity and Hydrogen Bond Strength and Their Coupling Effects.

Academic Credentials

Doctor of Philosophy:
Organization- Department of Chemistry, IIT Kanpur
Year- Jan, 2012 – June, 2018
Title of PhD Thesis: Quantification of Aromaticity and Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach
PhD Course Work: CGPA **8.00** out of **10**
(Best Thesis Award 2019 by Indian Society of Chemists and Biologists (ISCB), CSIR-CDRI, Lucknow)

Post Graduation:
University- M. Sc. in University of Lucknow
Year- 2008-2010
Subjects- Chemistry
Marks- 1049/1600 (**65.56%**)

Graduation:
University- B. Sc. in University of Lucknow
Year- 2005-2008
Subjects- Physics, Chemistry, Mathematics
Marks- 1199/1800 (**66.61%**)

Intermediate:
College- Adarsh Janta Inter College, Tanda, Ambedkar Nagar, Uttar Pradesh
Year- 2004
Subjects- Hindi (D), English, Physics (D), Chemistry, Mathematics (D)
Marks- 366/500 (**73.2%**)

High School:
College- Adarsh Janta Inter College, Tanda, Ambedkar Nagar, Uttar Pradesh
Year- 2002
Subjects- Hindi, English, Drawing (D), Science, Social Science, Mathematics (D)
Marks- 425/600 (**70.83%**)

Development

Development of Tools

1. **S. K. Pandey**, D. Manogaran, S. Manogaran, and H. F. Schaefer III, Quantification of Hydrogen Bond Strength Based on Interaction Coordinates (**HBSBIC**) (**2017**)
2. **S. K. Pandey**, D. Manogaran, S. Manogaran, and H. F. Schaefer III, Quantification of Aromaticity Based on Interaction Coordinates (**AIBIC**) (**2016**)

Patent(s)

1. S. Yadav, S. Awasthi, and **S. K. Pandey**, A method for the preparation of metal-nonmetal bonded PVA-Ni-D polymeric coating (Filing Date: 25/06/2025, Application No. **202521060787**, **Publication date: 18/07/2025**)
2. S. Awasthi, **S. K. Pandey**, H. J. Shwetha, Nehal, S. Selvaraj Durable Hydrogels, Process and Applications Thereof (Filing Date: 14/11/2024, Application No: **202411088023A**, **Publication Date: 29/11/2024**)
3. M. Goel, **S. K. Pandey**, M. Chawla, K. Singh. and N. Bhatnagar, Fabrication of high-performance symmetrical coin cell supercapacitors by using Poly (3,4-ethylenedioxythiphene): Polystyrene Sulfonate/Magnesium Oxide (PEDOT: PSS/MGO) Composite Electrodes (Filing Date: 02/09/2024, Application No: **202411066148**, Docket No: 123910, **Publication Date: 20/09/2024**).
4. A. Sharma, **S. K. Pandey**, D. Hans, H. Goel, A. K. Sisodia, C. Kumari, and Shivasharana CT, Device for on-site Detection with Power-Efficient Dye Sensitized Solar Cell Biosensor (Application No: **418260-001**) (Filing Date or CBR Date: 28/05/2024, **Publication date: 07/08/2024**, CBR No: 209181; Journal No: 32/2024; Journal Date: 09/08/2024).
5. S. Awasthi, C. Srivastava, M. S. Bobji, **S. K. Pandey**, and J. Gaur, Reinforced Hydrogel, Methods and Applications Thereof (Filing Date: Mar 24, 2022, Application No: **202241016585**, Publication Date: **22/07/2023**, and Grant Date: 11/03/2024).

Research Grants (s)

1. S. Prabhu (PI), **S. K. Pandey** (**Co-PI**), S. Awasthi (Co-PI), *Developing Polyacrylamide Hydrogel-Deferoxamine Based Nanocomposites to Target Ferroptosis-Induced Neurodegenerative Diseases,* Fetched MRB-Research Grant (**7.4 lacs**) through MAHE Bengaluru (grant used for 5 months, not availed due to switching from Manipal University Jaipur to NIT Bhopal)
2. S. Awasthi (PI) and **S. K. Pandey** (**Co-PI**), *Designing of High Strength, Strongly Bonded Hydroxyapatite Nanocomposite Coatings for Bone Repair***,** Fetched DST-Rajasthan Grant (**11.6 lacs**) (not availed due to switching from Manipal University Jaipur to NIT Bhopal)
3. **S. K. Pandey** (**PI**), *The Study on New Trapped Dimer Complexes (Hydrogen Versus Halogen Bond) Inside the C_{60} Cage, H-bonding/Aromaticity Coupling Effect, and Understanding the Phenomena of Cis- and Gauche Effects Using Compliance Constant and Interaction Coordinate Approaches*, Dr. D. S. Kothari – National Postdoctoral Fellowship (DSK-PDF) by UGC, New Delhi from Feb 2020 to Jan 2023 ~ **25 lacs**)

Project(s) Under Process

1. **S. K. Pandey** (**PI**), S. Awasthi, and K. D. Dubey, AI/ML-Driven *In Silico–In Vivo* Hybrid Platforms for Innovative Translational Development of Hydrogel Therapies in Soft Tissue Regeneration, Reference No.: **542025005397** (**ARG-ANRF**) **(~1 Cr)**
2. **S. K. Pandey** (**PI**) and S. Mukherjee (Co-PI), A concept proposal titled "In-Silico Probing on theTrapping of Rare Earth Elements in Fullerene andPrototype Systems and Their Potential Applications" (Resubmission Process) (**I-REL** (India) and RETTP Bhopal **2025**) (**40 lakh**).
3. **S. K. Pandey** (**Co-PI**), K. Pandey (**PI**), BIRAC Project (**5 Cr**) (Final round presentation and interaction completed) (**2025**) (Result awaited).
4. **S. K. Pandey** (**PI**) and S. Awasthi (Co-PI), A research proposal titled "Design and Surface Engineering of Layered Hydroxyapatite Coatings for Bone Regeneration: Interplay of Experiment and Theory" (Under Submission), (**MP-CST**, **2025**)
5. S. Awasthi (PI) and **S. K. Pandey** (**Co-PI**), A research proposal titled "Transition Metal Oxide Decorated Double-Layered Therapeutic Hydrogels for the Regeneration of Articular Cartilage and Healing of Diabetic Foot Ulcers" (Under Submission) (**DBT**, **2025**).

List of Publications (since 2015) *(Google Scholar Citations–1338; h-index-21 ; i10-index-42)*

1. M. Chauhan, Y. Budania, R. Mishra, A. Tyagi, P. Kumar, **S. K. Pandey***, S. Singh, Effect of Counter Electrode in Electrocatalytic Water Splitting Using FeO/NiO-Doped Graphitic Forest, Manuscript ID (ENERGYMATADV-D-25-00153), ***Energy Mat. Adv.*** [Published in affiliation with Beijing Institute of Technology (BIT) and published by the ***American Association for the Advancement of Science (AAAS)***] (**2025**), (***A Science Partner Journal, SPJ***) (Accepted on Oct 31, 2025) (**IF 15.9**, **Q1**, ISSN: 2692-7640)

2. N. Jakhar, M. Manohar, K. Arora, Ka. Balani, **S. K. Pandey*** and S. Awasthi, Nanoallotrope-Integrated Polyacrylamide Hydrogels: A Synergistic Experiment-Theory Approach for Engineering Mechanically Resilient and Cytocompatible Composites for Cartilage Tissue Regeneration, ***Nanoscale***, (Oct 20, **2025**), **DOI**: **10.1039/D5NR02168E** (**IF 6.7**, **Q1**, ISSN: 2040-3372, RSC)
3. S. Awasthi*, A. K. Pandey and **S. K. Pandey***, Mechanistic Insights into Intermolecular and Surface Interactions for Nanoscale Metal–Carbon-Based Coating Heterostructures, ***Coord. Chem. Rev.***, *543*, 216913, (Nov 15, **2025**), **DOI**: **10.1016/j.ccr.2025.216913** (**IF 23.5**). (**Q1**, Elsevier)
4. M. Goyal, **S. K. Pandey***, and N. Bhatnagar, Enhanced Electrochemical Activity of MgO Nanoparticles for High-Performance Supercapacitors, ***RSC Adv.***, 15, 25209-25220, (July 16, **2025**), **DOI: 10.1039/d5ra04329h** (**Q1**, RSC).
5. Vartika, **S. K. Pandey**, M. Pilania, Iodine-Mediated Synthesis of Indolyl-1,3,4-thiadiazole Amine Derivatives; Their DFT Analysis, ***RSC Adv.***, *15*, 156108, (May 23, **2025**) **DOI**: **10.1039/D5RA02026C** (**Q1**, RSC)
6. A. Yadav, V. K. Jain, V. Attatappa, N. Lakshmi, A Sharma, **S. K. Pandey***, and S. Awasthi, Effect of Temperature and Co-addition on Phase Stability, Magnetic and Electronic Properties of $Fe_{2-x}Co_xMnAl$ Quaternary Heusler Alloys for Spintronics Devices, ***J. Alloys Comp.*** *1027*, 180575, (May 10, **2025**) **DOI**: **10.1016/j.jallcom.2025.180579** (**Q1**, Elsevier)
7. M. Chauhan, Y. Budania, A. Modi, P. Kumar, **S. K. Pandey***, and S. Singh*, Trifunctional Nature of Heteroatom (B, N, S, O)-Doped Waste Diesel Soot: Turning Pollutants Into Potential Energy Catalysts for HER, OER, and ORR, ***Carbon Neutralization***, *4 (2)*, e195, (12 Feb, **2025**), **DOI: 10.1002/cnl2.195** (**IF 12**, **Q1**, Wiley)
8. A. Chakravorty, S. Das, A. A. Mini, S. Awasthi, **S. K. Pandey***, V. Raghavan, MXene-derived Potassium Titanate Nanoribbons Decorated Electrode Architecture for Detection of Ciprofloxacin: A Multipurpose Sensing Platform Development ***Mat. Adv.*** *6*, 2090-2109 (Feb 24, **2025**) **DOI: 10.1039/D4MA01245C** (**Q1**, RSC)
9. S. Awasthi, H. J. Shwetha, J. K. Gaur, and **S. K. Pandey***, Tough, Durable and Strongly Bonded Self-Healing Cartilage-mimicking Noncovalent Assembled Hydrogel Nanostructures: The Interplay between Experiment and Theory, ***Nanoscale*** *17*, 1616-1643, (Nov 21, **2024**) **DOI: 10.1039/D4NR03322A** (**IF 6.7**, **Q1**, ISSN: 2040-3372, RSC)
10. S. Yadav, **S. K. Pandey***, and S. Awasthi Particle surface engineering at the nano-micro scale interfaces of metal-nonmetal bonded polymeric coatings: experimental and *in silico* evaluation ***Nanoscale*** *17*, 1053-1068, (Nov 11, **2024**) **DOI**: **10.1039/D4NR03431G** (**Q1**, RSC)
11. S. Awasthi, B. P. Palomero, A. Srivastava and **S. K. Pandey***, Surface Functionalized Zinc Composite Coatings: A Review, ***Adv. Eng. Mat.*** *27 (2)*, 2401597, (Dec 16, **2024**) **DOI: 10.1002/adem.202401597** (**IF: 3.4**, **Q1**, Wiley)

12. L. Weng, M. Zhu, T. Gu, X. Liang, **S. K. Pandey**, H. Xu, R. Singhal, and G. D. Sharma Dimeric BODIPY Donors Based on the Donor–Acceptor Structure for all-small-molecule organic solar cells, ***ACS App. Energy Mat.*** *7 (23)*, 11195-11205, (Nov 26, **2024**), **DOI: 10.1021/acsaem.4c02425** (**Q1**, ACS)
13. S. Awasthi, A. Srivastava, D. Kumar, **S. K. Pandey***, N. M. Mubarak, M. H. Dehghani, and K. Ansari An insight into the toxicological impacts of carbon nanotubes (CNTs) on human health: A review, ***Env. Advances*** *18*, 100601, (**2024**), 100601 **DOI**: **10.1016/j.envadv.2024.100601** (**Q1**, Elsevier)
14. S. Awasthi, Komal and **S. K. Pandey***, Translational Applications of Magnetic Nanocellulose Composites, ***Nanoscale*** *16*, 15884, (July 30, **2024**), DOI: **DOI: 10.1039/D4NR01794C** (**IF 6.7**, **Q1**, ISSN: 2040-3372, RSC)
15. S. Das, A. Chakravorty, A. Raj, S. Luktuke, A. A. Mini, S. Awasthi, S. S. Sana, **S. K. Pandey*** and Vimala R. Graphene/MWCNT/Copper-Nanoparticle Fabricated Printed Electrode for Diclofenac Detection in Milk and Drinking Water: Electrochemical and DFT analysis, ***J. Mol. Liq.*** *411*, 125750, (Aug 12, **2024**) **DOI: 10.1016/j.molliq.2024.125750** (**IF: 6**, **Q1**, ISSN: 1873-3166, Elsevier)
16. A. Q. Malik, T. Jabeen, P. E. Lokhande, D. Kumar, S. Awasthi, **S. K. Pandey***, N. M. Mubarak, F. Abnisa, Molecularly imprinted Ag_2S quantum dots with high photocatalytic activity for dye removal: Experimental and DFT insights ***J. Environ. Manag.*** *366*, 121889, (July 24, **2024**) **DOI: 10.1016/j.jenvman.2024.121889** (**IF: 8.0**, **Q1**, ISSN: 1095-8630, Elsevier)
17. Amika, P. E Lokhande, R. U. Bhaskar, D. Kumar, S. Awasthi, and **S. K. Pandey***, Experimental and DFT Insights on Hydrothermally Synthesized PbS Doped Bismuth Titanate Perovskites: An Outperforming Photocatalytic Hydrogen Production Performance, ***Int. J. Hyd. Energy*** *78*, 534-546, (June 28, **2024**) **DOI: 10.1016/j.ijhydene.2024.06.217** (**IF: 7.2**, **Q1**, ISSN: 1879-3487, Elsevier)
18. M. Zhu, T. Gu, X. Liang, **S. K. Pandey**, C. P. Gros, H. J. Xu, and G. D. Sharma Small molecular donor materials based on β-β-bridged BODIPY dimers with triphenylamine or carbazole unit for efficient organic solar cells, ***Dalton Transaction*** *53*, 11981-11994, (June 14, **2024**) **DOI: 10.1039/D4DT01163E** (**IF: 4**, **Q1**, ISSN: 1477-9234, RSC)
19. S. Awasthi and **S. K. Pandey***, Recent advances in smart hydrogels and carbonaceous nanoallotropes composites, ***App. Mat. Today*** *36*, 102058/1-38, (Jan 13, **2024**) **DOI: 10.1016/j.apmt.2024.102058** (**IF: 8.3**, **Q1**, ISSN: 2352-9407, Elsevier)
20. S. Awasthi, S. De, and **S. K. Pandey***, Electrodeposited carbon nanostructured nickel composite coatings: A review, ***Heliyon*** *10 (8)*, e26051, (Feb 16, **2024**) **DOI: 10.1016/j.heliyon.2024.e26051** (**IF: 4**, **Q1**, ISSN: 2405-8440**,** Elsevier)
21. S. Awasthi, S. De, and **S. K. Pandey*** Advancement in Fabrication and Characterization Techniques of Nanocomposites, ***ACS Omega*** *9 (18)*, 19756–19769, (Apr 23, **2024**) **DOI: 10.1021/acsomega.3c09981** (**IF: 4.1**, **Q1**, ISSN: 2470-1343, ACS)

22. A. A. Mini, A. Chakravorty, S. Das, S. Awasthi, A. N. Grace, **S. K. Pandey***, and Vamala. R., CuO nanoparticles passivated 2D MXene-based voltammetric sensor for detecting environmental hazardous pollutant, ***Microchemical Journal*** *201,* 110648*,* (June 1, **2024**) **DOI:** **10.1016/j.microc.2024.110648** (**IF: 4.8**, **Q1**, ISSN: 1095-9149, Elsevier)
23. S. Awasthi, B. P. Palomero, A. Srivastava, S. Selvaraj, and **S. K. Pandey***, Nanodiamond-structured zinc composite coatings with strong bonding and high load-bearing capacity, ***Nanoscale Advances*** *6*, 1001-1010, (Jan 5, **2024**) **DOI:** **10.1039/D3NA00809F**. (**IF: 4.7**, **Q1**, ISSN: 2516-0230, RSC)
24. S. H. S. Pai, **S. K. Pandey**, E. J. J. Samuel, J. U. Jang. A. K. Nayak*, and H. S. Han, Recent advances in NiO-based nanostructures for energy storage device applications, ***J. Energy Storage*** *76 (15)*, 109731, (Jan 15, **2024**) **DOI:** **10.1016/j.est.2023.109731** (**IF: 9.4**, **Q1**, ISSN: 2352-1538, Elsevier)
25. T. Wei, T. Gu, X. Liang, H. Xu, G. Chayal, **S. K. Pandey**, and G. D. Sharma*, D-A-D type small molecule donors based on BODIPY skeleton for bulk heterojunction organic solar cells, ***J. Photochem. & Photobio. A: Chemistry*** *446*, 115103, (Jan 1, **2024**) **DOI:** **10.1016/j.jphotochem.2023.115103** (**IF: 4.3**, **Q1**, ISSN: 1873-2666, Elsevier)
26. A. R. Kumar, S. Selvaraj*, P. Rajkumar, J. Dhanalakshmi, M. Kumar, S. K. Nagarajan, P. Jayaprakash, G. P. S. Mol, S. Awasthi, and **S. K. Pandey*** Insights into structural, vibrational, and chemical shift characteristics, solvents impact (polar and nonpolar) on electronic properties and reactive sites, ADMET predictions, and ligand-protein interactions for antiviral drugs safrole and isosafrole: An *in-silico* approach, ***Chem. Phys. Impact*** *8*, 100443, (Dec 23, **2023**) **DOI:** **10.1016/j.chphi.2023.100443** (**IF: 2.2**, ISSN: 26670224, Elsevier)
27. S. K. Tiwari, **S. K. Pandey***, R. Randey, N. Wang, Y. K. Mishra*, M. Bystrzejewski, Y. Zhu, Stone-Wales Defect in Graphene, ***Small*** 2303340/1-32, (June 29, **2023**) **DOI**: **10.1002/smll.202303340** (**IF: 15.153**, **Q1**, ISSN: 1613-6829, Wiley)
28. A. R. Kumar, S. Selvaraj*, G. P. Mol, M. Selvaraj, L. Ilavarasan, **S. K. Pandey**, P. Jayaprakash, S. Awasthi, O. Albormani, and A. Ravi, Synthesis, solvent-solute interactions (polar and non-polar), spectroscopic insights, topological aspects, Fukui functions, molecular docking, ADME, and donor-acceptor investigations of 2-(trifluoromethyl)benzimidazole: A promising candidate for antitumor pharmacotherapy, ***J. Mol. Liq.*** *393*, 123661, (Nov 25, **2023**) **DOI:** **10.1016/j.molliq.2023.123661** (**IF: 6.0**, **Q1**, ISSN: 1873-3166, Elsevier)
29. T. Mandal, A. Ghosh, S. R. Mishra, **S. K. Pandey***, and V. Singh*, Development of Fluorescent Carbon Nanoparticles from Madhuca Longifolia Flower for Sensitive and Selective Detection of Cr (IV): A Collective Experimental-Computational Approach ***Nanoscale Adv.*** *5*, 4269, (July 18, **2023**) **DOI:** **10.1039/d3na00289f** (**IF: 5.598**, **Q1**, ISSN: 2516-0230, RSC)
30. **S. K. Pandey*** S. Hossain, and E. Arunan, New Insights into the Formation of CH_3OCH_3 and CH_3SCH_3 without and with the Assistance of Na^+ Ions and Some Implications for Interstellar Chemistry: An *In Silico* Approach, ***ACS Earth Space Chem.*** *7 (2)*, 388–403, (Feb 6, **2023**) **DOI**: **10.1021/acsearthspacechem.2c00292** (**IF: 3. 556**, **Q2**, ISSN: 2472-3452, ACS)

31. S. Das, A. Chakravorty, S. Luktuke, A. Raj, A. A. Mini, K. Ramesh, A. N. Grace, **S. K. Pandey*** and Vimala, R.*, Graphene/Gadolinium Oxide Composite Modified Screen-Printed Electrochemical Sensor for Detection of Diclofenac Sodium, ***Results in Chemistry*** *6*, 101189/1-8, (**2023**) **DOI: 10.1016/j.rechem.2023.101189** (**IF: 2.3**, ISSN: 2211-7156, Elsevier)
32. S. Awasthi, **S. K. Pandey***, J. Gaur, and C. Srivastava, Load Bearing Studies and Interfacial Interactions of Hydroxyapatite Composite Coatings for Bone Tissue Engineering, ***Mater. Chem. Front.*** *6 (24)*, 3731-3747, (**2022**) **DOI**: **10.1039/D2QM00898J** (**IF: 8.683**, **Q1**, ISSN: 2052-1537, RSC)
33. T. Wei, H. Dahiya, X. Liang, W. Zhu, **S. K. Pandey**, M. K. Singh, H. Xu, and G. D. Sharma*, Bulk heterojunction organic photovoltaic cells based on D-A type BODIPY small molecules as nonfullerene acceptor ***J. Mater. Chem. C*** *10 (35)*, 12776-12788, (**2022**) **DOI**: **10.1039/D2TC02497G** **IF: 8.067**, **Q1**, ISSN: 2050-7534, RSC)
34. X. Zong, H. Dahiya, Y. Song, X. Liang, **S. K. Pandey**, H. Xu, and G. D. Sharma*, Alkynyl BODIPY-Core Bridged Perylene Diimide Star-Shaped Nonfullerene Acceptors for Efficient Polymer Solar Cells, ***ACS Appl. Energy Mater.*** *5 (12)*, 15624-15637, (**2022**) **DOI**: **10.1021/acsaem.2c03200** (**IF: 6.959**, **Q1**, ISSN: 2574-0962, ACS)
35. **S. K. Pandey***, E. Arunan, R. Das, A. Roy, and A. K. Mishra, Recent advances in *in-silico* design and characterization of superalkali-based materials and their potential applications: A review ***Front. Chem.*** *10:1019166*, (**2022**) **DOI**: **10.3389/fchem.2022.1019166** (**IF: 5.545**, **Q1**, ISSN: 2296-2646, Frontiers)
36. R. S. S. S. Vemuri, **S. K. Pandey*,** and G. P. Khanal, A Computational Investigation on the Structural, Stability, and Electronic Feature Analyses of Substrates (Methyl Orange and Vanadium Oxide) Associated with Surfactant (Triton X-100), ***Curr. App. Poly. Sci.*** *5 (1)*, 60-71, (**2022**) **DOI: 10.2174/2452271605666220315155041** (ISSN: 2452-2724, Bentham Science)
37. S. Awasthi*, J. Gaur, **S. K. Pandey***, M. S. Bobji, and C. Srivastava, High Strength, Strongly Bonded Nanocomposite Hydrogels for Cartilage Repair ***ACS Appl. Mater. Interfaces*** *13 (21)*, 24505-24523, (**2021**). **DOI: 10.1021/acsami.1c05394** (**IF: 10.383**, **Q1**, ISSN: 1944-8252, ACS)
38. S. Awasthi*, **S. K. Pandey*,** E. Arunan and C. Srivastava, A Review on Hydroxyapatite Composites for Biomedical Application: From Experimental and Theoretical Perspectives, ***J. Mater. Chem. B*** *9 (2)*, 228-249, (**2021**) **DOI: 10.1039/D0TB02407D** (**IF: 7.571**, **Q1**, ISSN: 2050-7518, RSC) (Certified as a highly cited article by RSC)
39. **S. K. Pandey*** Novel and Polynuclear K- and Na-Based Superalkali Hydroxides as Superbases Better than Li-Related Species and Their Enhanced Properties: From *ab Initio* Exploration, ***ACS Omega*** *6 (46)*, 31077-31092, (**2021**) **DOI**: **10.1021/acsomega.1c04395** (**IF: 4.132**, ISSN: 2470-1343, ACS)
40. **S. K. Pandey***, Computational Study on the Structure, Stability, and Electronic Feature Analyses of Trapped Halocarbons inside a Novel Bispyrazole Organic Molecular Cage, ***ACS Omega*** *6 (17)*, 11711-11728, (**2021**) **DOI: 10.1021/acsomega.1c01019** (**IF: 4.132**, ISSN: 2470-1343, ACS)

41. P. Yadav, **S. K. Pandey**, P. Sharma, S. Kumar, M. Banerjee, and A. Sethi*, Experimental and Theoretical Investigation of synthesized Pregnenolone Derivatives via Palladium Catalyzed Cross Coupling Reactions, their anticancer activity against lung cancer cells, *J. Mol. Struct.* 1245, 131115, (**2021**) **DOI:** 10.1016/j.molstruc.2021.131115 (**IF: 3.841**, ISSN: 0022-2860, Elsevier)
42. **S. K. Pandey*** and E. Arunan, Effects of Multiple OH/SH Substitution on the H-bonding/Stability versus Aromaticity of Benzene Rings: From Computational Insights *Chemistry Select 6 (20)*, 5120-5139, (**2021**) **DOI:** 10.1002/slct.202100689 (**IF: 2.307**, ISSN: 2365-6549, Wiley)
43. S. Awasthi, **S. K. Pandey**, and K. Balani*, Tuning the Magnetism and Tribological Behaviour of Electrodeposited Ni/Cu Bi-layer by Selective Reinforcement of Carbon Nanotubes *J. Alloys Comp. 818*, 153287/1-12, (**2020**) **DOI:** 10.1016/j.jallcom.2019.153287 (**IF: 6.371**, ISSN: 0925-8388, Elsevier)
44. K. Singh*, A. Kumar, **S. K. Pandey**, S. Awasthi, S. K. Gupta, and P. Mishra, Interpretation of Adsorption Behaviour of Carboxymethyl Cellulose onto Functionalized Accurel Hydrophilic Polymeric Surface, *Ind. Eng. Chem. Res. 59 (43)*, 19102-19116, (**2020**) **DOI:** 10.1021/acs.iecr.0c03894 (**IF: 4.326**, ISSN: 1520-5045, ACS)
45. V. Mohan, N. Das, V. K. Jain, **S. K. Pandey**, Md. S. H. Faizi, J. Daniel, and P. Sen*, Highly Selective and Sensitive (PPB Level) Quinolin based Colorimetric Chemosensor for Cu(II) *Chemistry Select 5 (30)*, 9435-9442, (**2020**) **DOI:** 10.1002/slct.202001814 (**IF: 2.307**, ISSN: 2365-6549, Wiley)
46. R. K. Mudsainiyan*, A. K. Jassal, and **S. K. Pandey**, Structural Diversity from Co-crystal to 1D Coordination Polymers of 2, 6-NaphthaleneDicarboxylic Acid with 4, 4'-Bipyridine as Coligand: Structural and Computational Approach, *J. Coord. Chem. 73*, 3363-3381, (**2020**) **DOI:** 10.1080/00958972.2020.1853108 (**IF: 1.869**, ISSN: 0095-8972, Taylor & Francis)
47. S. Awasthi, **S. K. Pandey**, C. P. Pandey, and K. Balani*, Progress in Electrophoretic Deposition of Nickel with Carbonaceous Allotropes: A Review *Adv. Mater. Interfaces 7* (1), 1901096/1-33, (**2019**) **DOI:** 10.1002/admi.201901096 (**IF: 6.389**, ISSN: 2196-7350, Wiley)
48. K. Singh*, A. Kumar, S. Awasthi, **S. K. Pandey**, and P. Mishra, Adsorption Mechanism of Carboxymethyl Cellulose onto Mesoporous Mustard Carbon: Experimental and Theoretical Aspects, *Colloids and Surfaces A 581*, 123786 (**2019**) **DOI:** 10.1016/j.colsurfa.2019.123786 (**IF: 5.518**, ISSN: 0927-7757, Elsevier)
49. R. Singh, G. Kociok-Köhn, K. Singh, **S. K. Pandey***, and L. Singh, Influence of ligand coordination, solvent, and non-covalent interaction on the structural outcomes in coordination polymers with direct Cd(II)-alkanesulfonate bonds: A combined experimental and computational study *J. Solid State Chem. 280*, 120992, (**2019**) **DOI**: 10.1016/j.jssc.2019.120992 (**IF: 3.656**, ISSN: 0022-4596, Elsevier)
50. M. Gupta, K. Tomar, **S. K. Pandey**, and P. K. Bharadwaj*, Weak and Reversible Binding of Alkali Metal Ions (Na+/K+) by an Aza-Oxa Cryptand *Chemistry Select 4(5),* 1785-1788, (**2019**) **DOI:** 10.1002/slct.201803353 (**IF: 2.307**, ISSN: 2365-6549, Wiley)

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52. R. Singh, K. Singh, and **S. K. Pandey*,** A Computational Scrutiny on the Stability, Structural, and Electronic Features of Alkanesulfonate Based Zincate Salt with Varying Countercations ***Chemistry Select*** *3 (46)*, 13048-13056, (**2018**) **DOI:** 10.1002/slct.201803175 (**IF: 2.307**, ISSN: 2365-6549, Wiley)
53. M. Arora, S. K. Chawla, **S. K. Pandey**, and R. K. Mudsainiyan*, Anion Controlled Geometrically Different Cu(II) ion based Coordination Polymers and Green synthetic route for Copper nanoparticles: A Combined Experimental and Computational Insight ***J. Coord. Chem.*** *71 (14)*, 2243-2266, (**2018**) **DOI:** 10.1080/00958972.2018.1483077 (**IF: 1.869**, ISSN: 0095-8972, Taylor & Francis)
54. A. K. Srivastava, **S. K. Pandey*,** A. K. Pandey, N. Misra*, C_{60} as Electron Acceptor and Donor: A Comparative DFT Study of $Li@C_{60}$ and $F@C_{60}$ ***Aus. J. Chem.*** *71 (12)*, 953-956, (**2018**) **DOI:** 10.1071/CH18391 (**IF: 1.224**, ISSN: 0004-9425, CSIRO)
55. S. Awasthi, **S. K. Pandey**, A. Juyal, C. P. Pandey, and K. Balani*, Synergistic Effect of Carbonaceous Reinforcements on Microstructural**,** Electrochemical, Magnetic and Tribological Properties of Electrophoretically Deposited Nickel ***J. Alloys Comp.*** *711,* 424-433, (**2017**) **DOI:** 10.1016/j.jallcom.2017.04.003 (**IF: 6.371**, ISSN: 0925-8388, Elsevier)
56. A. K. Srivastava, N. Misra, and **S. K. Pandey***, DFT study on planar $(CaO)_n$ clusters (n = 1–5) and their hydrogen storage behavior ***J. Clust. Sci.*** *29 (1)*, 57-65, (**2017**) **DOI:** 10.1007/s10876-017-1306-x (**IF: 3.447**, ISSN: 1572-8862, Springer-Nature)
57. **S. K. Pandey**, D. Manogaran, S. Manogaran*, and H. F. Schaefer III, Quantification of Hydrogen Bond Strength Based on Interaction Coordinates: A New Approach ***J. Phys. Chem. A*** *121 (32)*, 6090-6103, (**2017**) **DOI:** 10.1021/acs.jpca.7b04752 (**IF: 2.944**, ISSN: 1089-5639, ACS)
58. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Structure, electronic properties and electronic excitation analyses of Si_{60}—Si_{60} dimer and $Si_{59}Al$—$S_{59}P$ complex ***Curr. App. Phys.*** *17 (11)*, 1376-1381, (**2017**) **DOI:** 10.1016/j.cap.2017.07.014 (**IF: 2.856**, ISSN: 1567-1739, Elsevier)
59. S. H. Mehdi, R. M. Ghalib, S. Awasthi, S. F. Alshahateet, R. Hashim, O. Sulaiman, and **S. K. Pandey***, Synthesis, Characterization, Crystal Structure, and Stability of 2-(5, 5-dimethyl-3-oxocyclohex-1-en-1-yl) Hydrazinecarbothioamide: A Combined Experimental and Theoretical Study ***Chemistry Select*** *2 (23)*, 6699-6709, (**2017**) **DOI:** 10.1002/slct.201700799 (**IF: 2.307**, ISSN: 2365-6549, Wiley)
60. R. K. Mudsainiyan and **S. K. Pandey**, A Combined Theoretical Calculations and Hirshfeld Surface Analysis of Cooperative Non-covalent Interactions in the Crystal Packing in $[Cu(L1)_2(EDA)]$ ***Z. Anorg. Allg. Chem.*** *643 (20)*, 1245-1252, (**2017**) **DOI:** 10.1002/zaac.201700182 (**IF: 1.414**, ISSN: 1521-3749, Wiley)
61. A. K. Srivastava, **S. K. Pandey** and N. Misra*, Structure, energetics, spectral and electronic properties of $B_3N_3C_{54}$ heterofullerene ***J. Nanostruct. Chem.*** *6*, 103-109, (**2016**) **DOI:** 10.1007/s40097-015-0184-8 (**IF: 8.00**, ISSN: 2193-8865, Springer-Nature)

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63. S. Sharma, G. Brahmachari*, B. Banerjee, K. Nurjamal, A. Kumar, A. K. Srivastava, N. Misra, **S. K. Pandey**, Rajnikant, and V. K. Gupta, Synthesis, spectroscopic characterization and crystallographic behavior of a biologically relevant novel indole-fused heterocyclic compound — Experimental and theoretical (DFT) studies ***J. Mol. Struct.*** *1118*, 344-355, (**2016**) **DOI: 10.1016/j.molstruc.2016.04.038** (**IF: 3.841**, ISSN: 0022-2860, Elsevier)
64. **S. K. Pandey**, D. Manogaran, S. Manogaran*, and H. F. Schaefer III, Quantification of Aromaticity Based on Interaction Coordinates: A New Proposal ***J. Phys. Chem. A*** *120 (18)*, 2894-2901, (**2016**) **DOI: 10.1021/acs.jpca.6b00240** (**IF: 2.944**, ISSN: 1089-5639, ACS)
65. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Stability *versus* aromaticity in mono-hydroxylated borazine, 1,2-azaborine and 1,3,2,4-Diazadiborine ***Mol. Phys.*** *114(11)*, 1763-1770, (**2016**) **DOI: 10.1080/00268976.2016.1145749** (**IF: 1.937**, ISSN: 0026-8976, Taylor & Francis)
66. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, BO_2 Functionalized $B_3N_3C_{54}$ Heterofullerene as a Possible Candidate for Molecular Spintronics and Nonlinear Optics ***Mater. Res. Exp.*** *3 (4)*, 045008/1-8, (**2016**) **DOI: 10.1088/2053-1591/3/4/045008** (**IF: 2.025**, ISSN: 2053-1591, IOP Science)
67. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, The aromaticity and electronic properties of monosubstituted benzene, borazine and diazaborine rings: An *ab initio* MP2 study ***Theor. Chem. Acc.*** *135*, 158/1-7, (**2016**) **DOI: 10.1007/s00214-016-1918-5** (**IF: 2.154**, ISSN: 1432-2234, Springer-Nature)
68. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, ($CH_3Br\cdots NH_3$)@C_{60}: The Effect of Nano Confinement on Halogen Bonding ***Chem. Phys. Lett.*** *662*, 240-243, (**2016**) **DOI: 10.1016/j.cplett.2016.09.036** (**IF: 2.713**, ISSN: 0009-2614, Elsevier)
69. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Prediction of Superalkali@C_{60} Endofullerenes, Their Enhanced Stability and Interesting Properties ***Chem. Phys. Lett.*** *655-656*, 71-75, (**2016**) **DOI: 10.1016/j.cplett.2016.05.039** (**IF: 2.713**, ISSN: 0009-2614, Elsevier)
70. A. K. Srivastava, A. Kumar, **S. K. Pandey**, and N. Misra*, Spectroscopic analyses, intra-molecular interaction, chemical reactivity and molecular docking of imerubrine into 5-HT3 receptor ***Med. Chem. Res.*** *25 (12)*, 2832-2841, (**2016**) **DOI: 10.1007/s00044-016-1710-z** (**IF: 2.351**, ISSN: 1054-2523, Springer-Nature)
71. **S. K. Pandey*,** M. F. Khan, S. Awasthi, R. Sangwan and S. Jain, A Quantum Theory of Atoms-in-Molecules Perspective and DFT Study of two Natural Products: Trans-communic and Imbricatolic Acid ***Aus. J. Chem.*** *70 (3)*, 328-333, (**2016**) **DOI: 10.1071/CH16406** (**IF: 1.224**, ISSN: 0004-9425, CSIRO)
72. **S. K. Pandey**, A. K. Srivastava, and N. Misra*, Relaxed Force Constants and QTAIM Analysis for Benzene, Borazine and Azaborines: New Insights into Bonding in the Six Membered Rings ***J. Comp. Meth. Mol. Des.*** *6*, 15-22, (**2016**) (ISSN: 2231-3176)

73. A. K. Srivastava, **S. K. Pandey**, A. Kumar, and N. Misra*, Vibrational Dynamics of B_3N_3 Substituted C_{60} Fullerene ***J. Sci. Res. Adv.*** *3*, 231-234, (**2016**) (ISSN: 2395-0226)
74. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Superhalogen properties of $ReF_n(n\geq6)$ species ***Chem. Phys. Lett.*** *624*, 15–18, (**2015**) **DOI:** 10.1016/j.cplett.2015.01.056 (**IF: 2.713**, ISSN: 0009-2614, Elsevier)
75. **S. K. Pandey**, P. Das, P. Das, E. Arunan, and S. Manogaran*, Intramolecular hydrogen bond: Can it be part of the basis set of valence internal coordinates in normal mode analysis? ***J. Chem. Sci.*** *127*, 1127-1134, (**2015**) **DOI:** 10.1007/s12039-015-0866-2 (**IF: 2.15**, ISSN: 0973-7103, Springer-Nature)
76. A. K. Srivastava, **S. K. Pandey**, S. K. Gangwar and A. Tamulis, Electronic transitions in two-micelle system: DFT and TD-DFT approaches ***J. Comp. Meth. Mol. Des.*** *5*, 27-32, (**2015**) (ISSN: 2231-3176)

Manuscript Under Revision (1)

77. M. Goyal, K. Singh, **S. K. Pandey*** and N. Bhatnagar Tailoring Supercapacitor Performance by Engineered PEDOT: PSS/MgO Nanohybrids with Zn and Cd Dopants **J. Power Sources** (**2025**) (**Q1**, *ISSN: 1873-2755,* Elsevier, **IF: 7.9**)

Manuscript Under Review (5)

78. S. Awasthi and **S. K. Pandey*** Zinc-Based Nanocomposites for Alzheimer's Therapy: Restoring Metal Homeostasis and Inhibiting Neurotoxic Protein Aggregation, ***Advanced Healthcare Materials*** (**2025**) (**IF 9.6, Q1**, ISSN: 2192-2659, Wiley).
79. S. Pareek, Komal, and **S. K. Pandey***, The Untapped Potential of Nanocellulose-Metal Oxide from Fibers to Smart Biohybrids: A Dual Experimental–Computational Lens, ***Nanoscale*** (**IF 6.7**, **Q1**, ISSN: 2040-3372, RSC)
80. D. Phogat, A. Srivastava, A. Goyal, **S. K. Pandey*** and S. Awasthi* Interface-Engineered Zn-HAP/hBN Composite Coatings with Hierarchical Control over Structural Integrity and Electronic Properties via Convergent Experimental and First-Principles Approaches ***J. Alloys. Comp.*** (July **2025**).
81. R. Jain, V. K. Jain, N. Lakshmi, A. Yadav, V. Jain, S. Kumawat, A. Sharma, S. Awasthi, and **S. K. Pandey***, Impact of Co Doping on the Magnetism and Electronic Structure of Fe_2MnSb Heusler Alloy: Insights from First-Principles Approach, ***Nanoscale*** (**2025**) (**IF 6.7**, **Q1**, ISSN: 2040-3372, RSC)
82. R. Singh, A. Tripathi, R. Kumar, M. Agarwal, and **S. K. Pandey*** First Computational Insight into Anionic, Neutral, and Cationic Supramolecular Motifs Featuring a Weak n-Propanesulfonate Ligand, ***Chem. Phys. Impact*** (Manuscript Number: CHPHI-D-25-00336) (**2025**) (Elsevier)

Manuscript Under Communication Process (6)

83. M. Goyal, **S. K. Pandey**, K. Singh, and N. Bhatnagar, Nanoarchitectured Zn-, Cd-, and Co-Doped MgO Nanoparticles with Augmented Electrodes Cell Conductivity for Energy Storage Applications, (**2025-26**)
84. R. Jain, V. K. Jain, N. Lakshmi, K. Soni, A. Jain, A. Sharma, S. Awasthi, and **S. K. Pandey***, Effect of Lattice Variation on Structural, Electronic and Magnetic Properties in $Fe_{2-x}Co_xMnSb$ using First Principal Calculation, (**2025-26**)

85. **S. K. Pandey***, Sukanya K. S., and E. Arunan, A Theoretical Study on Astatine/Iodine Mediated Halogen Bonding in Astatine Monoiodide with Some Selected Acceptors, (**2025-26**).
86. **S. K. Pandey***, A Computational Experiment on the Structure, Stability, and Electronic Properties of Free NH_3-HF, NH_3-HCl, NH_3-HBr, and NH_3-HI Dimer Complexes versus Their Encapsulation Inside C_{60} Cage (**2025-26**)
87. M. Goyal, S. Awasthi, N. Bhatnagar, and **S. K. Pandey***, Exploring the Potential of Lithium, Sodium, and Potassium Ion Batteries: A Review, (**2025-26**)
88. **S. K. Pandey*** Recent Progress in Quantifying Aromaticity Using Energetic, Structural, Electronic, and Magnetic Criteria: An Overview, (**2025-26**)

Manuscript Under Preparation (5)

89. **S. K. Pandey*** Recent Advances in *In-Silico* Design, Characterization, and Applications of Polyacrylamide Hydrogel-Based Biocomposites: A Mini-Review (**2026**)
90. K. Chandratre, P. Pragya, **S. K. Pandey**, B. P. Dhamaniya, P. Chhillar, S. Pathak, S. Karak, Development of perovskite inks for facile one-step coating of different morphologies, (**2026**)
91. **S. K. Pandey*** and R. Singh Computational Exploration of Anionic, Neutral, and Cationic Coordination Motifs Based on Weakly-coordinating n-propanesulfonate Anion (**2026**).
92. **S. K. Pandey*** and S. Manogaran, Interaction Coordinate Based Aromaticity for Some Five Membered Heterocyclic (X = O, N, and S) Systems and Their Protonated Analogs (**2026**).
93. **S. K. Pandey*** and S. Manogaran, Quantification of the Aromaticity for Some Fulvalene Systems Using Interaction Coordinate Approach (**2026**).

Book Editing/Authoring

1. **S. K. Pandey** (**Editor and Author**), S. Awasthi, A. Sharma, Meenakshi, R. Chaudhary, A. K. Pandey (**Co-editors**) **Book Title**: Quantum Dots: Advancing in Science and Engineering (**Taylor & Francis**) (Proposal Just Accepted) (July 24, **2025**)
2. **S. K. Pandey** (**Editor**) and S. Awasthi **Book Title:** Hierarchical Architectures in Coatings and Gels: Theory and Practice (**Elsevier**) (Proposal under review) (July 22, **2025**) (Ticket Number: 250722-022308)

Book Chapters (Published: 1, Accepted: 2, and Accepted (1)

Published (1)

1. S. Awasthi., S. De, and **S. K. Pandey***, **Book Chapter** - Chapter 25: Surface Grafting of Carbon Nanostructures, (**2024**) **Book Title**: Handbook of Composite Materials for Advanced Biomedical Application (**Springer-Nature**), 1-45, **DOI: 10.1007/978-3-031-14955-9_29-1**, **Print ISBN**: 978-3-031-14955-9

Accepted (2)

2. A. Srivastava, S. De, S. Awasthi, **S. K. Pandey***, **Book Title**: Sustainable Materials in Supercapacitors: New Developments in Green Energy Storage **Chapter 15**: Green

Supercapacitors in Transportation Systems (Accepted) (**2025**) (**Elsevier**)

3. M. Goel, S. Parashar, S. Awasthi, and **S. K. Pandey***, **Book title**: Handbook of Composite Materials for Advanced Biomedical Applications **Chapter 3**: Polymer Matrix Composites: Classifications and Therapeutic Applications. (Accepted), (**2025**) (**Springer-Nature**)

Book Chapter Proposal Accepted (1)

4. M. Goyal and **S. K. Pandey***, **Book title**: Quantum Dots: Advancing in Science and Engineering **Chapter 14**: Quantum Dots and Sustainability: A Framework for Safe Design and Regulatory Compliance, (**Taylor & Francis**) (July **2025**)

PhD Student(s)

1. Dipesh Gehlot since July 2025 (Supervisor)
2. Himanshu since July 2025 (Co-supervisor)
3. Mohnish Idpache, since Jan 2025 (Supervisor)
4. Bushra Nisa Khan, since July 2024 (Supervisor)

M.Sc. Student(s) (Dissertation Project and Presentation)

1. Mhd. Babar (Roll No 2320200102) (The student got an offer after two rounds of clearance from Akash Coaching Institute, Greater Noida, India: a 7.25 lakh annual package including a 3-lakh bonus) (Academic Session: Jan 2025 - June 2025) (Batch: 2023-2025).
2. Arsalan Tabrez (Roll No 2320200109) (The student got an offer after two rounds of clearance from Talent Trek Coaching Institute, Bengaluru, India; 8 lakhs annual package) (Academic Session: Jan 2025 - June 2025) (Batch: 2023-2025).
3. Pragati Dungrakoti (Roll No 24202001107) (Dissertation work is going on) (Academic Session: July 2025 - June 2026) (Batch: 2024-2026).
4. Deeksha Ghotki (Roll No 24202001114) (Dissertation work is going on) (Academic Session: July 2025 - June 2026) (Batch: 2024-2026).

U.G. Student(s) (Internship)

1. Vedant Mishra (Roll No: 24BCE10779, B.Tech., CSE, VIT Bhopal) 2025 (ongoing virtually)

2. Anisha Garg (Roll No: 24BAI10375, B.Tech., CSE (AI/ML), VIT Bhopal) 2025 (ongoing virtually)

Research Experience with Fellowship(s)

1. Serving as Assistant Professor in the Department of Chemistry, Maulana Azad National Institute of Technology Bhopal from Jan 9, 2024, till now.
2. Worked as Assistant Professor (Senior Scale) in the Department of Chemistry, Manipal University Jaipur, from Jan 27, 2023, to Jan 8, 2024.
3. Worked as Dr. D. S. Kothari - National Postdoctoral Fellow (DSK-PDF) Under University Grant Commission (UGC) Scheme, New Delhi, India from Feb 28, 2020, to Jan 26, 2023.
4. Under DST (Indo-French) Scheme, India for funding emolument (Postdoctoral Associate) from May 1, 2019, to Feb 27, 2020.

5. SERB under the Department of Science and Technology, India for funding emolument for the posts held as 'Project Scientist' from June 13, 2018, to April 30, 2019.
6. SERB under the Department of Science and Technology, India for funding emolument for the posts held as 'Senior Associate Researcher' from April 2, 2018, to June 12, 2018.
7. SERB under the Department of Science and Technology, India for providing stipend for the post held as 'Senior Research Fellow' from Feb 8, 2017, to April 1, 2018.
8. IIT Kanpur for providing emoluments for the post held as 'Senior Research Fellow' from Jan 1, 2017, to Feb 7, 2017.
9. UGC for facilitating the 'Senior Research Fellowship (SRF)' from Jan 1, 2014, to Dec 31, 2016, and 'Junior Research Fellowship (JRF)' from Jan 1, 2012, to Dec 31, 2013.

Teaching Experience and Interest

Currently Teaching

- ***At UG Level (B. Tech.)***

1. ***B.Tech.**: CY1110 – Environmental Science (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal).*
2. ***B.Tech.**: CY1126 – Engineering Chemistry Lab (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal)*

- ***At PG Level (M.Sc.)***

1. ***M.Sc.**: CY-MS-511 Quantum Chemistry and Basic Spectroscopy (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal).*
2. ***M.Sc.**: CY-MS-533 Instrumental Methods of Analysis (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal).*
3. ***M.Sc.**: CY-MS-515 Physical Chemistry Lab I and Minor Project I (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal).*
4. ***M.Sc.**: CHY-24615 Physical Chemistry Lab III (3rd Sem, July 2025 – Dec 2025, MANIT Bhopal).*
5. ***M.Sc.**: CHY-24618 Seminar III (3rd Sem, July 2025 – Dec 2025, MANIT Bhopal).*

- ***At Doctoral Level (PhD)***

1. *CHY812 – Advanced Physical Chemistry (1st Sem, Aug 2025 – Dec 2025, MANIT Bhopal).*

Teaching Experience (till now)

1. At UG Level (B.Sc. and B. Tech.)

1. ***B.Tech.**: CHY24126 – Engineering Chemistry Lab (2nd Sem, Jan 2025 – June 2025, MANIT Bhopal)*
2. ***B.Tech.**: CHY24110 – Environmental Science (2nd Sem, Jan 2025 – June 2025, MANIT Bhopal).*
3. ***B.Tech.**: CHY24126 – Chemistry Lab (1st Sem, July 2024 – Dec 2024, MANIT Bhopal)*
4. ***B.Tech.**: CHY24110 – Environmental Science (1st Sem, July 2024 – Dec 2024, MANIT Bhopal).*

5. ***B.Tech.**: CHY107 – Chemistry Lab (2nd Sem, Jan 2024 – May 2024, MANIT Bhopal)*
6. ***B.Tech.**: CHY106 – Environmental Chemistry (2nd Sem, Jan 2024 – May 2024, MANIT Bhopal).*
7. ***B.Sc.**: CY2160 – Analytical Chemistry Theory (3rd Sem, July 2023 – Dec 2023, Manipal University Jaipur).*
8. ***B.Sc.**: CY2138 – Analytical Chemistry Lab (3rd Sem, July 2023 – Dec 2023, Manipal University Jaipur).*
9. ***B.Tech.**: CY1001 – Engineering Chemistry (Theory and Lab) (1st Sem, July 2023 – Dec 2023, Manipal University Jaipur).*
10. ***B.Sc.**: CY1206 – Thermodynamics and Chemical Equilibrium (2nd Sem, Jan 2023 – May 2023, Manipal University Jaipur).*
11. ***B.Tech.**: CY1001 – Engineering Chemistry Theory (2nd Sem, Jan 2023 – May 2023, Manipal University Jaipur).*
12. ***B.Tech.**: CY1004 – Engineering Chemistry Lab (2nd Sem, Jan 2023 – May 2023, Manipal University Jaipur).*

At PG Level (M.Sc.)

1. ***M.Sc.**: CHY 24551 – Chemical and Statistical Thermodynamics (2nd Sem, Jan 2025 – May 2025, MANIT Bhopal).*
2. ***M.Sc.**: CHY 24525 - Physical Chemistry Lab II (2nd Sem, Jan 2025 – May 2025, MANIT Bhopal).*
3. ***M.Sc.**: CHY24528 – Seminar II (2nd Sem, Jan 2025 – May 2025, MANIT Bhopal).*
4. ***M.Sc.**: CHY621 – Project Dissertation and Presentation (4th Sem, Jan 2025 – May 2025, MANIT Bhopal).*
5. ***M.Sc.**: CHY654 – Photophysical Chemistry (3rd Sem, July 2024 – Dec 2024, MANIT Bhopal).*
6. ***M.Sc.**: CHY527 – Physical Chemistry Lab II (2nd Sem, Jan 2024 – May 2024, MANIT Bhopal).*
7. ***M.Sc.**: CHY24518 – Seminar I (1st Sem, July 2024 – Dec 2024, MANIT Bhopal).*
8. ***M.Sc.**: CHY614 – Chemistry Lab III (3rd Sem, July 2024 – Dec 2024, MANIT Bhopal).*
9. ***M.Sc.**: CHY24527 – Physical Chemistry Lab II (2nd Sem, July 2024 – Dec 2024, MANIT Bhopal).*
10. ***M.Sc.**: CHY521 – Chemical Kinetics and Thermodynamics (2nd Sem, Jan 2024 – May 2024, MANIT Bhopal).*
11. ***M.Sc.**: CHY527 – Physical Chemistry Lab (2nd Sem, Jan 2024 – May 2024, MANIT Bhopal).*
12. ***M.Sc.**: CY6202 – Analytical Chemistry and Bonding (2nd Sem, Jan 2022 – May 2023, Manipal University Jaipur).*
13. ***M.Sc.**: CY6109 – Advanced Physical Chemistry (1st Sem, July 2023 – Dec 2023, Manipal University Jaipur).*

At Doctoral Level (PhD.)

1. *CHY811 – Research Methodology (2nd Sem, Jan 2025 – June 2025, MANIT Bhopal).*

- ***Teaching Assistance (TA)/Other Related Experiences***

1. **One and half year's** teaching experience in a coaching at **B. Sc** (Honors and JAM levels) and **M. Sc** levels during July - 2010 to November 2011.
2. **More than five years** teaching experiences as a TA at IIT Kanpur at **UG** (B. Tech., B.S., Dual, and Integrated) and **PG** (**M.Sc.** - GATE, CSIR-UGC NET-JRF, and BARC) Level Exams during Ph.D. tenure at IIT Kanpur.
3. **CHM101A** Introductory Chemistry Lab (**2014-2015, 1st Semester**) and **CHM102A** General Chemistry (Physical Chemistry - Theory) (**2014-2015, 2nd Semester**) and **CHM102A** General Chemistry (Quantum Chemistry) (**2015-2016, 2nd Semester**).

Achievements, Honors, and Awards

1. **First prize** in '**Best Oral Presentation 2021**' at an international conference during Jul 14-16, 2021, by J. C. Bose University of Technology and Science Faridabad.
2. Selected for the **Young Scientist Award Presentation** in the 'Young Scientist Award Program 2019-20' by the **Indian Science Congress Association (ISCA), New Delhi, Govt. of India** during Jan 3-7, 2020.
3. Qualified **CSIR-UGC (NET and JRF)** 2011.
4. Qualified **GATE** in 2011.
5. Cracked **OCES/DGFS** in 2011 and 2013 organized by BARC.
6. **Best Thesis Award 2019** in "25th ISCB International Conference (ISCBC-2019) Trends in Chemical and Biological Sciences: Impact on Health and Environment" organized by **CSIR-CDRI Lucknow** during Jan 12-14, 2019.
7. **Bharat Jyoti Award – 2019** by Indian International Friendship Society, India, New Delhi is given by Honorable Former Chief Justice Permod Kohli of High Court Sikkim dated March 28, 2019.
8. **Best Research Award 2018** in National Student Research Convention - 2018 organized by **IIT Kanpur** during Mar 9-11, 2018.
9. **First prize** in '**Best Oral Presentation 2015**' delivered at the National Symposium on Innovative Methods in Chemistry Education organized by the Department of Chemistry, the **University of Lucknow,** during Oct 8-10, 2015.
10. **First prize** in '**Best Poster Presentation 2016**' in Research Scholar Day organized by the Department of Chemistry, **IIT Kanpur** on Feb 27, 2016.
11. **Young Scientist Award 2018** as an appreciation in Chemistry at the "International Conference on Chemical Sciences: National and Global Perspective" at Lucknow, Christian College, the **University of Lucknow** during Oct 29-31, 2018.
12. **Young Scientist Award 2018** in Chemistry through the "Venus International Research Awards (VIRA-2018) by the Centre for Advanced Research and Design (CARD) of Venus International Foundation (VIF) during the Annual Research Meet (ARM-2018) on Aug 11, 2018.
13. **Research Leadership Award of the Year 2020** (Innovative Scientist in Electronic Structure Calculations – Computational Chemistry) by **World Research Council (WRC)** on Jan 26, 2020.

Invited Talk in Conferences/Seminar/Workshop/Symposium

1. Invited talk at Sunway University organized by the Research Centre for Nanomaterials and Energy Technology (RCNMET), Sunway University Malaysia on June 3, 2025.
2. Given hands-on training on an STTP in AMRIT 2025 organized by the Department of Chemistry, MANIT Bhopal, during July 23-27, 2025.
3. Given hands on training on the Computational Chemistry Labs (Session 1 and Session 2) in a National Workshop (Short Term Course) on the "Interpretation of Instrumentation Methods in Science and Engineering (IIMSE-2025)" organized by the Department of Chemistry, MANIT Bhopal during Mar 24-28, 2025.
4. Invited Talk at an Internation Conference on "Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems (PCAMC-2024)" organized by the Department of Chemistry, IISER Kolkata during 11-14 Dec 2024.
5. Invited talk in an International Conference on Multidisciplinary Approaches to Chemical Sciences (InCoMACS 2024) organized by the Department of Chemistry, National P. G. College Lucknow during Oct 24-26, 2024.
6. Invited talk to an "Expert Resource Person" in a national workshop "Advanced Computational Chemistry Workshop 2024", organized by the Department of Chemistry, VIT Bhopal during 17-18 Oct 2024.
7. Invited Lecture in "Lucknow Climate Change Conference on Control of Greenhouse Gases at the Source by Physical and Chemical Technology (LCCCCGGSPCT_2k22)" Organized by Department of Chemistry, School of Physical & Decision Sciences (SPDS), Babasaheb Bhimrao Ambedkar University (A Central University) Lucknow during April 22-24, 2022.
8. Invited for 'Young Scientist Award Talk' under the Young Scientists Award Program in Indian Science Congress Association (ISCA) conference organized by ISCA during Jan 3-7, 2020.
9. Invited Talk in "Global Conference on the Control of Greenhouse Gases at the Source by Physical and Chemical Technology (GCGHGSPCT-2019)" Organized by Department of Chemistry, School of Physical & Decision Sciences (SPDS), Babasaheb Bhimrao Ambedkar University (A Central University) Lucknow during April 22-24, 2019.
10. Invited Talk as "Young Scientist" in "International Symposium on Advances in Functional & Biological Materials (ISAFBM - 2019)" Organized by Humboldt Academy Lucknow and Physics Department, University of Lucknow on Feb 28, 2019 on the Occasion of National Science Day.
11. Invited Talk as "Young Scientist" in "International Conference on Chemical Sciences: National and Global Prospective" at Lucknow Christian College, University of Lucknow, during Oct 29-31, 2018.
12. Invited Talk on "87th Birth Anniversary Seminar on Dr. A. P. J. Abdul Kalam" at BBAU, Lucknow (A Central University) during Oct 15-16, 2018.

Paper presented in Conferences/Seminar/Workshop

International

1. Oral Talk in International Conference (Virtual) on Recent Advancements in Chemical Sciences – 2021, organized by the Department of Chemistry, J. C. Bose University of Science & Technology, Faridabad, during Jul 14-16, 2021.
2. Presented a Paper in "India International Science Festival (IISF) 2019" on the theme "Frontier Area of Research" held at Biswa Bangla Convention Centre, Kolkata, during Nov 5-8, 2019.
3. Oral Talk in "Indian Society of Chemists and Biologists (ISCB) 25th ISCB International Conference (ISCBC-2019)" on "Trends in Chemical and Biological Sciences: Impact on Health and Environment" in Chemical Sciences organized by "CSIR-CDRI Lucknow" during Jan 12-14, 2019.
4. Presented Poster at "IUPAP conference on Computational Physics" held at IIT Guwahati during Dec 2-5, 2015.
5. Presented Poster in "Theoretical Chemistry Symposium - 2014" organized by "CSIR-National Chemical Laboratory, Pune" during Dec 18-21, 2014.
6. Presented Poster in "International Symposium Dynamics of Complex Chemical and Biological Systems" held at IIT Kanpur during Feb 13-15, 2014.
7. Presented Poster at "International Conference on Bimolecular Simulations and Dynamics: 2013 Recent Advances and Future Perspectives" at IIT Madras during Nov 28-30, 2013.

National

8. Oral Talk in "National Conference on Chemical Sciences: Advancing Frontiers" (NCCSAF - 2019)" Organized by the Department of Chemistry, the University of Lucknow during Mar 15-16, 2019.
9. Oral Talk in "National Student Research Convention – 2018" organized by "IIT Kanpur" during Mar 9-11, 2018.
10. Presented Paper in "1st National Virtual Conference on Scientific Research and Advances (VCSRA)" organized by the "VCSRA Community" during Feb 20-25, 2018.
11. Presented Poster at "National Symposium on Innovative Methods in Chemistry Education" organized by the "Department of Chemistry, University of Lucknow" during Oct 8-10, 2015.
12. Oral Talk at "National Symposium on Innovative methods in Chemistry Education" organized by the "Department of Chemistry, the University of Lucknow" during Oct 8-10, 2015.
13. Presented Paper at "5th National Conference on Nanotechnology and Material Science" held at the Department of Physics, the University of Lucknow during Dec 21-23, 2013.

Institute/University/College

14. Presented Poster at "Research Scholar Day – 2016" organized by the "Department of Chemistry, IIT Kanpur" on Feb 27, 2016.
15. Presented Poster in "Royal Society of Chemistry Symposium – 2015" organized by the "Department of Chemistry, IIT Kanpur" on Nov 23, 2015.

16. Presented Poster in "Student Research Convention – 2014" at IIT Kanpur held during Aug 9-10, 2014.

Offline-Online Conference/Workshop/Seminar Organized or Admin Roles Therein (4)

1. National Advisory Committee for 'Technovation 2025' organized by Career Point Kota University during Dec 14-15 2025.
2. An External Expert in the Doctoral Committee (DC) meeting for a PhD scholar of the Department of Chemistry, VIT Bhopal, on 17th Oct 2024.
3. Advisory Committee Member for an International Conference on Multidisciplinary Approaches to Chemical Sciences (InCoMACS 2024) organized by the Department of Chemistry, National P. G. College Lucknow, during 24-26 Oct 2024.
4. Role as a **Convenor** in an "Online Webinar Series 2023" on "Blending of Forensic Science with Law - Crime Spot to Court Room" organized by the **Department of Chemistry** and the Department of Law, Manipal University Jaipur dated on June 2, 2023. Title of the Talk: "Issues and Perspectives of Forensic Document Examination"; Guest Speaker: Professor Pàvlos G. Kipouràs, Judicial and Professional Graphologist, *University of Thrace,* Greece.
5. Role as a **Convenor** in an "Online Webinar Series 2023" on "Blending of Forensic Science with Law - Crime Spot to Court Room" organized by the **Department of Chemistry** and the Department of Law, Manipal University Jaipur dated on June 19, 2023. Title of the Talk: "*Admissibility of Evidence in Criminal Court: an international overview*"; Guest Speaker: Dr. Eugenio D'Orio, Director General, *Bioforensics Research Centre*, Italy.

Research Professional Role (s)

1. Guest Editor of **Discover Applied Science** (Computational Chemistry sections) of Springer-Nature (Impact Factor: **2.8**) from Sep 2025.
2. Editorial Board Member in the '***Journal of Composites and Biodegradable Polymers***' (***ISSN**: 2311-8717*), ***Savvy Science Publisher***, China.
3. Editorial board member of '**Discover Molecules**' journal of the ***Springer-Nature*** publisher. https://link.springer.com/journal/44345/editorial-board
4. Review Editor of **Frontiers in Chemistry** (Theoretical and Computational Chemistry section) (Impact Factor: **5.221**) from Feb 3, 2021. https://loop.frontiersin.org/people/1221781/overview
5. Review Editor of **Frontiers in Physics** (Physical Chemistry Chemical Physics & Theoretical and Computational Chemistry sections) (Impact Factor: **3.718**) from April 2022. https://loop.frontiersin.org/people/1221781/overview
6. Executive Guest Editor of **Current Applied Polymer Science** (**CAPS**) published by Bentham Science publishers from Dec 18, 2020, to June 2025.

Membership (s)

1. **Associate Member** (AM: AASCT39) of **The Asian Association of Sugar Cane Technologists (AASCT), Lucknow** since Sep 27, 2021.
2. Member of the **Materials Research Society of India (MRSI)** (Membership No: **LMB3297**) from Jan 18, 2021.
3. Member of the **Indian Science Congress Association (ISCA)** (Membership No: **L38300**) from July 15, 2019.
4. Member of the **Prof. H. S. Srivastava (PHSS) Foundation for Society and Science** (Membership No: **PHSFS-LP8**) from Nov 12, 2018.
5. Member of the **Indian Society of Chemists and Biologists (ISCB)** (Membership Fellow Number: **LF-882/18**) from July 9, 2018.
6. Member of the **American Chemical Society (ACS)** (Membership Number: **31022128**) since 2017.
7. Member of the **Association of Chemistry Teachers (ACT)** (Membership No: **1772**) from Nov 23, 2015.

Participated in Seminar/Conference/Workshop

1. Participated in an International Conference on Water Future Conference: Towards a Sustainable Water Future Organized by Divecha Centre of Climate Change & Sustainable Water Future Programme Hosted by Indian Institute of Science during Sep 24-27, 2019.
2. Participated in "4th Annual Research Meet-ARM2018" organized by the "Centre for Advanced Research and Design (CARD)" of "Venus International Foundation (VIF)" on Aug 11, 2018 in Chennai.
3. Participated in a national seminar "Mini Colloquium on Nanoelectronics" organized by the "IEEE Electron Devices Society, Uttar Pradesh Chapter and the Department of Electrical Engineering" at IIT Kanpur on Aug 26, 2017.
4. Participated in "Introduction to Gaussian: Theory and Practice Workshop" organized by "SCUBE Scientific Software Solutions and Gaussian, Inc. Researcher" during Jan 16-20, 2017.
5. Participated in "ACS Reviewer Lab Training" organized by "American Chemical Society Community and Department of Chemistry, IIT Kanpur" on Jan 13, 2017.
6. Participated in "National Seminar on Ancient India Science and Technology" held at IIT Kanpur on Oct 14, 2015.
7. Participated in "National Symposium on Radiation and Photochemistry" at IIT Kanpur during Mar 9-11, 2015.
8. Participated in "Summer Radio Workshop - 2014" organized by "Media Technology Centre, IIT Kanpur" during May 20-25, 2014.
9. Participated in "Seminar on Organometallic Chemistry" organized by "Special Assistance Program (UGC) and Department of Chemistry, University of Lucknow" on Mar 31, 2010.

10. Spirited participation/contribution in "Training Workshop of Model Rocketry" at PMS Degree College, Lucknow organized by "Voluntary Institute for Community Applied Science" during Mar 21-24, 2009.

News/Media (Via Channel/News Paper/Website)

➢ Research highlights entitled "Catalysts from vehicle exhaust soot help generate hydrogen - Conversion method can reduce air pollution" published in scientific media (**Nature India**) dated on **27/03/2025**.
https://www.nature.com/articles/d44151-025-00047-9

➢ Research news entitled "Turning pollution into power: New method transforms carbon nanoparticles from emissions into renewable energy catalysts" came in Science Media PHYS.ORG (**Nanotechnology - Nanomaterials**) dated on **03/03/2025.**
https://phys.org/news/2025-03-pollution-power-method-carbon-nanoparticles.html

➢ Research news entitled "Innovative Method Converts Carbon Nanoparticles into Electrocatalysts" came in media (**Life Technology - Nanomaterials**) dated on **03/03/2025.**
https://www.lifetechnology.com/blogs/life-technology-science-news/innovative-method-converts-carbon-nanoparticles-into-electrocatalysts?srsltid=AfmBOor0QSkblVh1qHlEwJiFi_jQ7pn9dKjtDc_lfv214scun3ZqH2MY

➢ Research news entitled "Innovative Method Converts Carbon Nanoparticles into Electrocatalysts" came in social media (on Facebook under **Nanomaterials – Computational Studies blog published by Quantum Server Networks**) dated on **04/03/2025.**
https://www.facebook.com/groups/184031292131597/posts/1858809844653725/?_rdr

➢ Research news entitled "Turning pollution into power: New method transforms carbon nanoparticles from emissions into renewable energy catalysts" came in media (on X.com platform) dated on **04/03/2025.**
https://x.com/judithcallagha9/status/1896661496488165836

➢ Research work came in media (ETV Bharat – National News Channel) for designing a novel biomaterial used in cartilage repair (biomedical) applications through interview held in the lab dated on **31/07/2021**.
https://www.etvbharat.com/english/national/bharat/iisc-develop-high-strength-hydrogels-for-cartilage-repair/na20210731101743882

➢ A research highlights on the work related to ***Cartilage Repair (ACS Applied Materials & Interfaces)*** was published by IISc News on IISc main website on 20th July **2021**. *https://iisc.ac.in/cartilage-repair-using-high-strength-hydrogels/*

➢ News highlighted in Dainik Jagran Ambedkar Nagar (a small district in Uttar Pradesh) for milestone research on Feb 28, 2021 on the **Occasion of National Science Day**.

➢ A biography was published by Dainik Jagran Ambedkar Nagar, Uttar Pradesh for outstanding research regarding **Best Thesis Award 2019** at **international** level.

➢ A solo biography was highlighted by Dainik Jagran Ambedkar Nagar, Uttar Pradesh for best research activities (**Young Scientist Award 2018**).

➢ **Young Scientist Award 2018** (**International**) as an appreciation was published by Dainik Jagran Ambedkar Nagar, Uttar Pradesh on 7th Nov 2018.

➢ A prestigious achievement, **Bharat Jyoti Award** honored by *Former Chief Justice (Permod Kohli) of the Hon'ble High Court of Sikkim, New Delhi* through IIFS, New Delhi was published by Dainik Jagran, Ambedkar Nagar, Uttar Pradesh in **2019**.

Social Networking Sites for Scientific Community

Google Scholar ID: https://scholar.google.com/citations?user=HS5n4_4AAAAJ

Scopus ID: 57204434951

Web of Science (Researcher ID): X-9935-2018

ResearchGate ID: https://www.researchgate.net/profile/Sarvesh-Pandey

ORCID iD: https://orcid.org/0000-0002-6315-8118

Vidwan-ID: 610626

LinkedIn: https://www.linkedin.com/in/dr-sarvesh-kumar-pandey-4ba3bba1/

Scientific and Computational Experiment Skills

- ***Computational Chemistry:*** *Execution of my two developed tools,* ***AIBIC 2016*** *for the quantification of Aromaticity and* ***HBSBIC 2017*** *for the quantification of hydrogen bond strength.*
- ***Software Tool Exposure****: NCI-plot, Multiwfn, Avogadro, VMD, Chemcraft, Chemdraw, CrystalExplorer, Diamond, Gabedit, GaussView, Jmol, Mercury, Molden, and Vesta Expertise in MS-Office, Excel, Experience in Windows and Linux operating systems, search engines like SciFinder, Reaxys, Scopus, and Web of Science.*
- ***Gaussian*** *for* ***Quantum Chemical (Electronic Structure) Calculations****.*

- ***AIMAll*** *for study of several topological parameters of structural and electronic properties of the chemical as well as biological systems in* ***Quantum Theory of Atoms in Molecules (QTAIM)***
- *Some other useful tools (AI/ML, GROMACS, and Quantum ESPRESSO packages).*
- ***Language Skill:*** *English has been the medium of instruction throughout my academic carrier, and I can fluently speak and write in this language. Besides this, I have a good knowledge of Hindi as a regional language.*

Professional (Research Papers/Books Review) Academic Activities (more than 40)

1. Reviewed a research article for **Diamond and Related Materials** in Oct 2025.
2. Reviewed a research article for **ACS Omega** in September 2025 (11/09/2025).
3. Reviewed a research article for ***Polycyclic Aromatic Compounds*** in July 2025.
4. *Reviewed a research article for* ***ChemistrySelect*** *(Wiley) in June 2025.*
5. *Reviewed a research article for* ***J. Mat. Chem. B*** *(RSC) in April 2025.*
6. *Reviewed a book chapter for the* ***Advancements in Comp.-Aided Drug Discovery and Development: A Comprehensive Overview*** *(Bentham Science) (Reference: BMS-FICC-2024-HT1-1257-20) in Sep 2024.*
7. *Reviewed a research article for the* ***J. Inorg. and Organomett. Poly. and Mat.*** *(Springer-Nature) in Sep 2024.*
8. *Reviewed a research article for the* ***Analyt. Methods*** *(RSC) in Sep 2024.*
9. *Reviewed a research article for the* ***J. Mol. Liq.*** *(Elsevier) in June 2024.*
10. *Reviewed a research article for the* ***ACS Omega*** *(ACS) in May 2024.*
11. *Reviewed a research article in* ***Comput. and Theoret. Chem.*** *(Elsevier) in Apr 2024.*
12. *Reviewed 4 research articles for the* ***Front. in Chem.*** *(Theoretical and Computational Chemistry) in Nov 2021, Feb 2022, April 2022, and July 2022.*
13. *Reviewed 4 research articles for* ***Main Group Chem.*** *in Oct 2015, May 2018, and July 2021, April 2022, and July 2022.*
14. *Reviewed a research article for* ***J. Cluster Sci.*** *in Aug 2017.*
15. *Reviewed a research article for* ***Aus. J. Chem.*** *in Dec 2017.*
16. *Reviewed a research article for* ***ChemistrySelect*** *in 2018.*
17. *Reviewed 5 research articles for the* ***Curr. Comp.-Aided Drug Design*** *(****CC-ADD****) in Jan 2019, Mar 2019, Sep 2019, Jan 2020, Mar 2020.*
18. *Reviewed a research article for the* ***Int. J. Comp. Theoret. Chem.*** *in Feb 2019.*
19. *Reviewed a research article for the* ***J. Dispersion Sci. Tech.*** *in Mar 2020.*
20. *Reviewed 4 research articles for the* ***Spectrochimica Acta Part A: Mol. Biomol. Spectroscopy*** *in May 2019, Aug 2020, Aug 2021, and June 2023, respectively.*
21. *Reviewed 2 research articles for the* ***Curr. Pharmaceutical Biotech. (CPB)*** *in Aug 2020.*
22. *Reviewed a research article for the* ***Ind. J. Chem*** *in May 2020.*

23. *Reviewed a research article for the **Chiang Mai J. Sci.** in Jan 2020.*
24. *Reviewed a communication paper for the **Chem. Phys. Lett.** in Sep 2020.*

Extra-Curricular Activities

1. *Played a role (in preparing draft) in the MoU between the MANIT Bhopal and University of Lorraine, France.*
2. *Played the role of one of the core representatives for three foreign delegates (Asian Development Bank-ADB, Philippines and South Korea) and two Indian delegates (one from the ADB and the Ministry of Education, India) during their visit and discussion related to **the Research Park Project** (~50 Cr) at MANIT Bhopal.*
3. *Worked as a Volunteer in "The Salters' Chemistry Camp" organized by the Salters' Institute in collaboration with the Royal Society of Chemistry as part of the Inspirational Chemistry Programme, sponsored by Dr. Yusuf Hamied, leading Indian philanthropist and pioneer in the pharmaceutical industry, at the Indian Institute of Technology Kanpur during Nov 30 –Dec 2, 2018.*
4. *Worked as **Buddy**, Counselling Service, PG Wing, **IIT Kanpur** during **2016-2017**.*
5. *Worked as a **Mentor**, Counselling Service, PG Wing, **IIT Kanpur** during **2015-2016**.*
6. *Worked as an **Orientation Team Member**, Counselling Service, PG Wing, **IIT Kanpur** during **2014-2015**.*
7. *Worked as an **Orientation Team Member**, Counselling Service, PG Wing, **IIT Kanpur** during **2013-2014**.*
8. *Worked as **Maintenance Secretary** of **Hall-7, IIT Kanpur,** during **2014-2015**.*
9. *Worked as **Anti Anti-Noise Committee Member** of **Hall-7, IIT Kanpur** during **2012-2013**.*
10. *Worked as **Maintenance Committee Member** of the **Hall-7, IIT Kanpur** during **2012-2013**.*
11. *Worked as **Volunteer** of Hall Day of the **Hall-7, IIT Kanpur** during **2012-2013**.*
12. *Worked as **Cultural Committee Member** of the **Hall-7, IIT Kanpur** during **2013-2014**.*
13. *Worked as **Volunteer** of Hall Day of the **Hall-7, IIT Kanpur** during **2013-2014**.*
14. *Participated in **10 KM MARATHON** and **completed successfully** organized by **Adventure Club, Games and Sports Council, IIT Kanpur** on **Mar 15, 2015**.*
15. *Participated in **Blood Donation Camp** organized by **G. S. V. M. Medical College, Kanpur in IIT Kanpur** in **Nov 1, 2014**.*

Academic Contributions to the Department/Institute

1. *Faculty coordinator for interaction of B.Tech 1st year students with a start-up founder, VyomGARUD UAV Solutions, dated on Nov 17, 2025.*
2. *Faculty coordinator for interaction of B.Tech 1st and 2nd Year students with BIRAC coordinator, Central India, dated on Nov 7, 2025.*

3. *Faculty I/C in the procurements of the P-XRD instrument since Oct 18, 2025.*
4. *Convenor of the 'Modifications in Existing Feedback System' of the MANIT Bhopal since Oct 17, 2025, to till now.*
5. *Coordinator for the 'Swachchhatta Pakhwara Awarness' Program from E-Cell, ROLTA Incubation Centre, MANIT Bhopal Dated on Sep 27, 2025 (Saturday).*
6. *Coordinator for the MSME-related Hackathon 2026 competition on Aug 19, 2025.*
7. *Warden of Hostel 3 (A. P. Kanvinde Bhawan), MANIT Bhopal, from June 13, 2025, till now.*
8. *Mentor of one start-up (Tri-V) student (Mr. Jai Soni from the Mechanical Engineering Department) in the ROLTA Incubation Centre, MANIT Bhopal.*
9. *Coordinator of E-Summit 2025, organized by E-Cell, ROLTA Centre, MANIT Bhopal, during Feb 14-16, 2025.*
10. *Co-coordinator of NASHA MUKT BHARAT ABHIYAN (NMBA) committee in Hostel 3* (A. P. Kanvinde Bhawan)*, MANIT Bhopal.*
11. *Secretary of the ROLTA Incubation Centre, MANIT Bhopal, since Aug 21, 2024.*
12. *Core Committee Member of ROLTA Incubation Centre, MANIT Bhopal, since July 10, 2024.*
13. *Assistant Warden of Hostel 3 (A. P. Kanvinde Bhawan), MANIT Bhopal, from July 8, 2024, to June 12, 2025.*
14. *Served as Assistant Warden of Hostel 1 (Homi Jahangir Bhabha Hostel), MANIT Bhopal, from Feb 16, 2024, to July 7, 2024.*
15. *Co-convenor of E-Summit 2024, organized by E-Cell, ROLTA Centre, MANIT Bhopal during Feb 9-11, 2024.*
16. *UG Purchase Committee Member (Chemicals, Glassware, and Equipment) in the Chemistry Department.*
17. *ERP Coordinator of the Department of Chemistry since June 1, 2024.*
18. *Worked as a Coordinator of "Industry Connect" in the Department of Chemistry, Manipal University, Jaipur.*
19. *Worked as a Co-coordinator of M.Sc. (Chemistry) Program in the Department of Chemistry, Manipal University Jaipur (2023-2025).*
20. *Played the lead role in a summer camp organized by the Department of Chemistry, Manipal University, Jaipur, dated May 11, 2023.*
21. *Worked as an Admission Committee Member (B.Sc. and M.Sc.) for 2023-24 (Manipal University Jaipur).*
22. *Academic Administration and Mentoring at the department level (Chemistry Department) and institute level (IIT-Kanpur), setting up Labs and Quiz, Mid Semester, and End-semester exams.*

Personal Skills

- *Ability to work in a new and challenging environment.*
- *Good organizing skills and interpersonal skills and have willingness to work in groups and ability to lead group activities.*
- *Hardworking and very eager to learn new concepts, ideas and use new technologies.*
- *Strong planning and coordinating abilities and having attitude to share information and new knowledge.*
- *Motivated, efficient, resourceful, and reliable and have a positive thinking in every situation.*
- *To do something better for human beings.*
- Warm and friendly as a person.

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