

Bio-Data

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Current Position: Assistant Professor

Organization - Department of Chemistry, National Institute of Technology (NIT) Bhopal, Bhopal – 462 003, Madhya Pradesh, India

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Subject – Physical/Materials Chemistry

Specialization - Computational Chemical and Materials Science (Electronic Structure Calculations) and Diverse Interesting Parameters Validating to Experimental Facets

Current Area of Research Interest

- **Computational Materials Science**

- *In-Silico* Design and Characterization of Novel Materials (Inorganic/Organic) and their Potential Applications.
- Theoretical Elucidation of Interfacial Interaction(s) Involved in Smart Biocomposites based on Hydrogels (like PAM), Ceramics (like HAP), *etc.*
- Understanding and Uncovering Features of Newly Designed Small Complexes Associated with Carbonaceous Materials (Fullerene, CNT, Graphene, Diamond, *etc.*) using the Molecular Surgery Approach.

- **Computational Astrochemistry**

- Attain New Insights and Unraveling the Formation of Diverse Chemical and Biological Species by Possible Formation Pathways through Concerted (Single Step)/Intermediate (Multistep) Molecular Reaction Mechanisms in the Interstellar Medium (ISM).

- **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/Research Credentials

Postdoctoral/Post-PhD Experiences

Organization – Department of Inorganic and Physical Chemistry, IISc Bengaluru

Organization – Department of Chemistry, IIT Kanpur

Doctor of Philosophy

Organization- Department of Chemistry, IIT Kanpur

Title of PhD Thesis: Quantification of Aromaticity and Hydrogen Bond Strength

Based on Interaction Coordinates: A New Approach

(**Best Thesis Award 2019 by Indian Society of Chemists and Biologists (ISCB), CSIR-CDRI, Lucknow**)

Graduation (B.Sc.) and Post-Graduation (M.Sc.)

University - University of Lucknow

High School and Intermediate

School/College - Adarsh Janta Inter College, Tanda, Ambedkar Nagar, Uttar Pradesh

Developed Tools

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

Patents

1. S. Awasthi, C. Srivastava, M. S. Bobji, **S. K. Pandey**, and J. Gaur, Reinforced Hydrogel, Methods and Applications Thereof (Ref No/Application No: **202241016585**) (Filing Date: Mar 24, 2022, Publication Date: 22 July 2023, and Grant Date: 11 March 2024).
2. A. Sharma, **S. K. Pandey**, D. Hans, H. Goel, A. K. Sisodia, C. Kumari, and S. CT Device for on-site Detection with Power-Efficient Dye Sensitized Solar Cell Biosensor (Application No: **418260-001**) (Filing Date: May 28, 2024, **CBR No: 209181**) (Under Review).

Projects

- ❖ S. Awasthi (PI) and **S. K. Pandey** (Co-PI), A research proposal titled “Designing of High Strength, Strongly Bonded Hydroxyapatite Nanocomposite Coatings for Bone Repair” (Result Awaited) (May, **2024**) (**CST-DST Rajasthan**).
- ❖ Vimala R. (PI) and **S. K. Pandey** (Co-PI), Development of MXene Based Printed Electrochemical Aptasensor for Detection of Pesticide: Combined *In-Silico* and Experimental Approach (**Proposal Under Submission Process, CRG-SERB, DST 2024**)
- ❖ **S. K. Pandey** (PI) and S. Awasthi (Co-PI), Design and Characterization of Functionalized Polyacrylamide (PAM) based Biocomposite Allied with Metal and Ceramic for Biomedical Application (**Proposal Under Submission Process in the CST-DST, MP, 2024**)

List of Publications (since 2015) (Google Scholar Citations till now: 717)

1. 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, (2023) DOI: [10.1002/smll.202303340](https://doi.org/10.1002/smll.202303340) (IF: 15.153, ISSN: 1613-6829, Wiley)
2. 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, (2024) DOI: [10.1016/j.est.2023.109731](https://doi.org/10.1016/j.est.2023.109731) (IF: 9.4, ISSN: 2352-1538, Elsevier)
3. S. Awasthi* and **S. K. Pandey***, Recent advances in smart hydrogels and carbonaceous nanoallotropes composites, *App. Mat. Today* 36, 102058/1-38, (2024) DOI: [10.1016/j.apmt.2024.102058](https://doi.org/10.1016/j.apmt.2024.102058) (IF: 8.3, ISSN: 2352-9407, Elsevier)
4. 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 (2024) 110648, DOI: [10.1016/j.microc.2024.110648](https://doi.org/10.1016/j.microc.2024.110648) (IF: 4.8, ISSN: 1095-9149, Elsevier)
5. 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, (2024) DOI: [10.1039/D3NA00809F](https://doi.org/10.1039/D3NA00809F). (IF: 4.7, ISSN: 2516-0230, RSC)
6. 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, (2024) DOI: [10.1016/j.jphotochem.2023.115103](https://doi.org/10.1016/j.jphotochem.2023.115103) (IF: 4.3, ISSN: 1873-2666, Elsevier)
7. S. Awasthi*, S. De, and **S. K. Pandey*** Advancement in Fabrication and Characterization Techniques of Nanocomposites, *ACS Omega*, 9 (18), 19756–19769, (2024) DOI: [10.1021/acsomega.3c09981](https://doi.org/10.1021/acsomega.3c09981) (IF: 4.1, ISSN: 2470-1343, ACS)
8. S. Awasthi*, S. De, and **S. K. Pandey***, Electrodeposited carbon nanostructured nickel composite coatings: A review, *Heliyon*, 10 (8), e26051, (2024) DOI: [10.1016/j.heliyon.2024.e26051](https://doi.org/10.1016/j.heliyon.2024.e26051) (IF: 4, ISSN: 2405-8440, Elsevier)
9. 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 safrrole and isosafrole: An *in-silico* approach, *Chem. Phys. Impact* 8, 100443, (2024) DOI: [10.1016/j.chphi.2023.100443](https://doi.org/10.1016/j.chphi.2023.100443) (IF: 2.2, ISSN: 26670224, Elsevier)
10. 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, (2023) DOI: [10.1016/j.molliq.2023.123661](https://doi.org/10.1016/j.molliq.2023.123661) (IF: 6.0, ISSN: 1873-3166, Elsevier)

11. 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, (2023) DOI: [10.1039/d3na00289f](https://doi.org/10.1039/d3na00289f) (IF: 5.598, ISSN: 2516-0230, RSC)
12. **S. K. Pandey*** S. Hossain, and E. Arunan, New Insights into the Formation of CH₃OCH₃ and CH₃SCH₃ 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, (2023) DOI: [10.1021/acsearthspacechem.2c00292](https://doi.org/10.1021/acsearthspacechem.2c00292) (IF: 3.556, ISSN: 2472-3452, ACS)
13. 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](https://doi.org/10.1016/j.rechem.2023.101189) (IF: 2.3, ISSN: 2211-7156, Elsevier)
14. 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](https://doi.org/10.1039/D2QM00898J) (IF: 8.683, ISSN: 2052-1537, RSC)
15. 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](https://doi.org/10.1039/D2TC02497G) IF: 8.067, ISSN: 2050-7534, RSC)
16. 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](https://doi.org/10.1021/acsaem.2c03200) (IF: 6.959, ISSN: 2574-0962, ACS)
17. **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](https://doi.org/10.3389/fchem.2022.1019166) (IF: 5.545, ISSN: 2296-2646, Frontiers)
18. 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](https://doi.org/10.2174/2452271605666220315155041) (ISSN: 2452-2724, Bentham Science)
19. 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/acsaami.1c05394](https://doi.org/10.1021/acsaami.1c05394) (IF: 10.383, ISSN: 1944-8252, ACS)
20. 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](https://doi.org/10.1039/D0TB02407D) (IF: 7.571, ISSN: 2050-7518, RSC)

21. **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](https://doi.org/10.1021/acsomega.1c04395) (IF: 4.132, ISSN: 2470-1343, ACS)
22. **S. K. Pandey***, Computational Study on the Structure, Stability, and Electronic Feature Analyses of Trapped Halocarbons inside a Novel Bispirazole Organic Molecular Cage, *ACS Omega* 6 (17), 11711-11728, (2021) DOI: [10.1021/acsomega.1c01019](https://doi.org/10.1021/acsomega.1c01019) (IF: 4.132, ISSN: 2470-1343, ACS)
23. 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](https://doi.org/10.1016/j.molstruc.2021.131115) (IF: 3.841, ISSN: 0022-2860, Elsevier)
24. **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](https://doi.org/10.1002/slct.202100689) (IF: 2.307, ISSN: 2365-6549, Wiley)
25. 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](https://doi.org/10.1016/j.jallcom.2019.153287) (IF: 6.371, ISSN: 0925-8388, Elsevier)
26. 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](https://doi.org/10.1021/acs.iecr.0c03894) (IF: 4.326, ISSN: 1520-5045, ACS)
27. 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](https://doi.org/10.1002/slct.202001814) (IF: 2.307, ISSN: 2365-6549, Wiley)
28. 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](https://doi.org/10.1080/00958972.2020.1853108) (IF: 1.869, ISSN: 0095-8972, Taylor & Francis)
29. 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](https://doi.org/10.1002/admi.201901096) (IF: 6.389, ISSN: 2196-7350, Wiley)
30. 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](https://doi.org/10.1016/j.colsurfa.2019.123786) (IF: 5.518, ISSN: 0927-7757, Elsevier)

31. 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](https://doi.org/10.1016/j.jssc.2019.120992) (IF: 3.656, ISSN: 0022-4596, Elsevier)
32. 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](https://doi.org/10.1002/slct.201803353) (IF: 2.307, ISSN: 2365-6549, Wiley)
33. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, A Computational Study on Semiconducting Si₆₀, Si₅₉Al and Si₅₉P Nanocages *Chem. Phys. Lett.* 691, 82-86, (2018) DOI: [10.1016/j.cplett.2017.11.001](https://doi.org/10.1016/j.cplett.2017.11.001) (IF: 2.713, ISSN: 0009-2614, Elsevier)
34. 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 Counteranions *Chemistry Select* 3 (46), 13048-13056, (2018) DOI: [10.1002/slct.201803175](https://doi.org/10.1002/slct.201803175) (IF: 2.307, ISSN: 2365-6549, Wiley)
35. 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](https://doi.org/10.1080/00958972.2018.1483077) (IF: 1.869, ISSN: 0095-8972, Taylor & Francis)
36. A. K. Srivastava, **S. K. Pandey***, A. K. Pandey, N. Misra*, C₆₀ as Electron Acceptor and Donor: A Comparative DFT Study of Li@C₆₀ and F@C₆₀ *Aus. J. Chem.* 71 (12), 953-956, (2018) DOI: [10.1071/CH18391](https://doi.org/10.1071/CH18391) (IF: 1.224, ISSN: 0004-9425, CSIRO)
37. 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](https://doi.org/10.1016/j.jallcom.2017.04.003) (IF: 6.371, ISSN: 0925-8388, Elsevier)
38. 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](https://doi.org/10.1007/s10876-017-1306-x) (IF: 3.447, ISSN: 1572-8862, Springer-Nature)
39. **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](https://doi.org/10.1021/acs.jpca.7b04752) (IF: 2.944, ISSN: 1089-5639, ACS)
40. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Structure, electronic properties and electronic excitation analyses of Si₆₀—Si₆₀ dimer and Si₅₉Al—Si₅₉P complex *Curr. App. Phys.* 17 (11), 1376-1381, (2017) DOI: [10.1016/j.cap.2017.07.014](https://doi.org/10.1016/j.cap.2017.07.014) (IF: 2.856, ISSN: 1567-1739, Elsevier)
41. 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](https://doi.org/10.1002/slct.201700799) (IF: 2.307, ISSN: 2365-6549, Wiley)

42. 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)
43. A. K. Srivastava, [S. K. Pandey](#) and N. Misra*, Structure, energetics, spectral and electronic properties of B₃N₃C₅₄ heterofullerene *J. Nanostruct. Chem.* 6, 103-109, (2016) DOI: [10.1007/s40097-015-0184-8](#) (IF: 8.00, ISSN: 2193-8865, Springer-Nature)
44. A. K. Srivastava, [S. K. Pandey](#) and N. Misra*, Encapsulation of lawrencium into C₆₀ fullerene: Lr@C₆₀ versus Li@C₆₀ *Mater. Chem. Phys.* 177, 437-441, (2016) DOI: [10.1016/j.matchemphys.2016.04.050](#) (IF: 4.778, ISSN: 0254-0584, Elsevier)
45. 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)
46. [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)
47. 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)
48. A. K. Srivastava, [S. K. Pandey](#), and N. Misra*, BO₂ Functionalized B₃N₃C₅₄ 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)
49. 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)
50. A. K. Srivastava, [S. K. Pandey](#), and N. Misra*, (CH₃Br...NH₃)@C₆₀: 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)
51. A. K. Srivastava, [S. K. Pandey](#), and N. Misra*, Prediction of Superalkali@C₆₀ 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)
52. 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)

53. **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: Transcommunic and Imbricatolic Acid *Aus. J. Chem.* 70 (3), 328-333, (2016) DOI: [10.1071/CH16406](#) (IF: 1.224, ISSN: 0004-9425, CSIRO)
54. **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)
55. A. K. Srivastava, **S. K. Pandey**, A. Kumar, and N. Misra*, Vibrational Dynamics of B₃N₃ Substituted C₆₀ Fullerene *J. Sci. Res. Adv.* 3, 231-234, (2016) (ISSN: 2395-0226)
56. A. K. Srivastava, **S. K. Pandey**, and N. Misra*, Superhalogen properties of ReF_n(n≥6) species *Chem. Phys. Lett.* 624, 15–18, (2015) DOI: [10.1016/j.cplett.2015.01.056](#) (IF: 2.713, ISSN: 0009-2614, Elsevier)
57. **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)
58. A. K. Srivastava, **S. K. Pandey**, S. K. Gangwar and A. Tamulis, Electronic transitions in two micelles system: DFT and TD-DFT approaches *J. Comp. Meth. Mol. Des.* 5, 27-32, (2015) (ISSN: 2231-3176)

Manuscript Revision Submitted (2)

59. 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, *Jnt. J. Hyd. Energy*, (Manuscript ID: HE-D-24-00010.R1) (Minor Revision Submitted) (May, 2024) (IF: 7.2, ISSN: 1879-3487, Elsevier).
60. 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* (Manuscript No.: DT-ART-04-2024-001163) (Major Revision submitted) (May, 2024) (IF: 4, ISSN: 1477-9234, RSC).

Manuscript Received for Revision (1)

61. A. Q. Malik, P. E. Lokhande, D. Kumar, S. Awasthi, **S. K. Pandey***; N. M. Mubarak, Molecularly Imprinted Ag₂S Quantum Dots with High Photocatalytic Activity for Dye Removal: Experimental and DFT Insights, *J. Env. Manag.* (Manuscript No.: JEMA-D-24-00647) (Major Revision under Submission Process) (May, 2024) (IF: 8.7, ISSN: 1095-8630, Elsevier).

Manuscript under Review (8)

62. S. Yadav, **S. K. Pandey***, and S. Awasthi* Experimental and *In-Silico* Evaluations on the Synergistic Effect of Metallization and Carbonaceous Reinforcements Towards Strength and Bonding of Polymeric Coatings *Reports on Progress in Physics (ROPP)* (Under Review) (Manuscript ID: ROPPR-100289) (2024) (IF: 18.1, ISSN: 1361-6633, IOP)

63. M. Chauhan, Y. Budania, A. Modi, P. Kumar, [S. K. Pandey*](#), and S. Singh Unlocking the synergic effect of heteroatoms (B, N, S, O) doped HER, OER, and ORR via wet and DFT experiments, *J. Mat. Chem. A* (Manuscript ID: TA-ART-05-2024-003363), (2024), (Under Review), (IF: 11.9, ISSN: 2050-749, RSC)
64. S. Awasthi, Komal and [S. K. Pandey*](#), Translational Applications of Magnetic Nanocellulose Composites, *Nanoscale* (Manuscript ID: NR-REV-04-2024-001794), (Under Review) (2024), (IF 6.7, ISSN: 2040-3372, RSC)
65. S. Awasthi, [S. K. Pandey*](#), H. J. Shwetha and J. K. Gaur, Tough, Durable and Strongly Bonded Self-Healing Cartilage-mimicking Noncovalent Assembly Hydrogel Nanostructures: The Interplay of Experiment and Theory, *Nanoscale* (Manuscript ID: NR-ART-05-2024-001912), (2024) (IF 6.7, ISSN: 2040-3372, RSC),
66. 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.* (Manuscript No.: MOLLIQ-D-24-04467), (Under Review), (2024), (IF: 6, ISSN: 1873-3166, Elsevier)
67. M. Goyal, [S. K. Pandey*](#), K. Singh, and N. Bhatnagar, Nanoarchitected Zn-, Cd-, and Co-Doped MgO Nanoparticles with Augmented Electrodes Cell Conductivity for Energy Storage Applications, *Mat. Chem. Phys.*, (2024) (IF 4.6, ISSN: 1879-3312, Elsevier)
68. S. Awasthi*, B. P. Palomero, A. Srivastava and [S. K. Pandey*](#), A Review on Surface Modifications of Zinc Composite Coatings by Selective Reinforcements, *J. Mat. Sci.* (Manuscript ID: JMSC-D-24-02807), (2024) (IF 4.5, ISSN: 1573-4803, Elsevier)
69. S. Awasthi*, A. Srivastava and [S. K. Pandey*](#), Carbon Nanotubes Toxicity: A Review on Consequences and Remedies, *Mat. Today Comm.* (Manuscript ID: MTCOMM-D-24-05611), (2024) (IF 3.8, ISSN: 2352-4928, Elsevier)

Manuscript Under Pipeline for Communication (4)

70. [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, *Chem. Comm.* (Invited article for submission) (2024). (IF: 6.065, ISSN: 1364-548X 1948-7185, RSC)
71. [S. K. Pandey*](#), A Computational Experiment on the Structure, Stability, and Electronic Properties of Free NH₃-HF, NH₃-HCl, NH₃-HBr, and NH₃-HI Dimer Complexes versus the Their Encapsulation Inside C₆₀ Cage *J. Phys. Chem. Lett.* (Invited article for submission) (2024) (IF: 5.7, ISSN: 1948-7185, ACS)
72. M. Goyal, S. Awasthi, N. Bhatnagar, and [S. K. Pandey*](#), Exploring the Potential of Lithium, Sodium, and Potassium Ion Batteries: A Review, (2024)
73. [S. K. Pandey*](#) Recent Progress in Quantifying Aromaticity Using Energetic, Structural, Electronic, and Magnetic Criteria: An Overview, (2024)

Manuscript under Preparation (5)

74. [S. K. Pandey*](#) Recent Advances in In-Silico Design, Characterization, and Applications of Polyacrylamide Hydrogel Based Biocomposites: A Mini-Review (2024)

75. 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, (2024)
76. **S. K. Pandey*** and R. Singh Computational Exploration of Anionic, Neutral, and Cationic Coordination Motifs Based on Weakly-coordinating n-propanesulfonate Anion (2024).
77. **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 (2024).
78. **S. K. Pandey*** and S. Manogaran, Quantification of the Aromaticity for Some Fulvalene Systems Using Interaction Coordinate Approach (2024).

Book Chapters (Published: 1 and Under Review: 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](https://doi.org/10.1007/978-3-031-14955-9_29-1), Print ISBN: 978-3-031-14955-9
2. A. Srivastava, S. De, S. Awasthi., **S. K. Pandey***, Chapter 15: Green Supercapacitors in Transportation Systems (**Chapter Under Review Process**) (Nov, 2023)
Book Title: Sustainable Materials in Supercapacitors: New Developments in Green Energy Storage (**Elsevier**)

PhD Student(s)

Sakshi Pareek, Designing advanced biomass driven nanocomposites for wastewater treatment: Harmonizing theory and practice, Supervisor (Dr. Komal Arora, Manipal University Jaipur) and **Co-supervisor** (**Dr. S. K. Pandey**, MANIT Bhopal)

Research Experience with Fellowships

1. Worked as D. S. Kothari - National Postdoctoral Fellow (DSK-NPDF) Under University Grant Commission (UGC) Scheme, New Delhi, India from Feb 28, 2020 to Feb 27, 2023.
2. Under DST (Indo-French) Scheme, India for funding emolument (Postdoctoral Fellow as RA-Level II) from May 1, 2019 to Feb 27, 2020.
3. 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 and 'Project Scientist' from June 13, 2018 to April 30, 2019.
4. 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.
5. IIT Kanpur for providing emolument for the post held as 'Senior Research Fellow' from Jan 1, 2017 to Feb 7, 2017.
6. 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

▪ **At UG Level (B.Sc. and B. Tech.)**

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

▪ **At PG Level (M.Sc.)**

1. **M.Sc.:** CHY521 – Chemical Kinetics and Thermodynamics (2nd Semester, Jan 2024 – May 2024, MANIT Bhopal).
2. **M.Sc.:** CHY527 – Physical Chemistry Lab (2nd Semester, Jan 2024 – May 2024, MANIT Bhopal).
3. **M.Sc.:** CY6202 – Analytical Chemistry and Bonding (2nd Semester, Jan 2022 – May 2023, Manipal University Jaipur).
4. **M.Sc.:** CY6109 – Advanced Physical Chemistry (1st Semester, July 2023 – Dec 2023, Manipal University Jaipur).

▪ **Teaching Assistantship (TA)/Other Teaching Experiences**

5. **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.
6. **More than five years** teaching experiences as a TA at **UG** and **PG** Levels (B. Tech., B.S., Dual, and Integrated)
7. **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**).
8. **More than five years** teaching experiences as a TA at **PG** level (**M.Sc.** - GATE, CSIR-UGC NET-JRF, and BARC level) during Ph.D. tenure at IIT Kanpur.

Achievements, Fellowship, 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. **D. S. Kothari – Postdoctoral Fellowship (DSK–PDF)** on Feb 28, 2020.
3. 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.
4. Qualified **CSIR-UGC (NET and JRF)** 2011.
5. Qualified **GATE** in 2011.
6. Cracked **OCES/DGFS** in 2011 and 2013 organized by BARC.
7. **Best Thesis Award 2019** in "25th ISCB International Conference (ISCB-2019) Trends in Chemical and Biological Sciences: Impact on Health and Environment" organized by **CSIR-CDRI Lucknow** during Jan 12-14, 2019.
8. **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.
9. **Best Research Award 2018** in National Student Research Convention - 2018 organized by **IIT Kanpur** during Mar 9-11, 2018.
10. **First prize in 'Best Oral Presentation 2015'** delivered at National Symposium on Innovative methods in Chemistry Education organized by the Department of Chemistry, the **University of Lucknow** during Oct 8-10, 2015.
11. **First prize in 'Best Poster Presentation 2016'** in Research Scholar Day organized by the Department of Chemistry, **IIT Kanpur** on Feb 27, 2016.
12. **Young Scientist Award 2018** as an appreciation in Chemistry at the "International Conference on Chemical Sciences: National and Global Prospective" at Lucknow Christian College, the **University of Lucknow** during Oct 29-31, 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 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.
2. 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.
3. Invited Talk in "Global Conference on the Control of Greenhouse Gases at the Source by Physical and Chemical Technology (GCGHGPCT-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.

4. 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.
5. 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.
6. 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 Conference/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 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 (ISCB-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.

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 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 highlight 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.
- **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&hl=en

Scopus ID: [57204434951](https://www.scopus.com/authid/detail.uri?authorid=57204434951)

Web of Science Researcher ID: [X-9935-2018](https://www.webofscience.com/wos/author/uri?uri=wsn:0009-9935-2018)

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

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

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

Scientific and Computational Experiment Skills

- **Computational Chemistry:** Execution of two developed tools, **AIBIC 2016** for the quantification of Aromaticity and **HBSBIC 2017** for the quantification of hydrogen bond strength.
- **Software Tools 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 Software (Quantum EXPRESSO, GAMESS, and MOLPRO package under learning process)

Membership/Editorial Board Member

1. Editorial board member of 'Discover Molecules' journal of Springer-Nature publishing house.
2. Review and Guest Editor of **Frontiers in Chemistry** (Theoretical and Computational Chemistry) (Impact Factor: **5.221**) from Feb 3, 2021. <https://loop.frontiersin.org/people/1221781/overview>
3. 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>
4. Executive Guest Editor of **Current Applied Polymer Science (CAPS)** published by Bentham Science publishers since Dec 18, 2020. <https://benthamscience.com/journal/166/editorial-board>
5. **Associate Member of The Asian Association of Sugar Cane Technologists (AASCT), Lucknow** (AM: AASCT39) since Sep 27, 2021.
6. Member of the **Materials Research Society of India (MRSI)** (Membership No: **LMB3297**) from Jan 18, 2021.
7. Member of the **Indian Science Congress Association (ISCA)** (Membership No: **L38300**) from July 15, 2019.
8. Member of the **Prof. H. S. Srivastava (PHSS) Foundation for Society and Science** (Membership No: **PHSFS-LP8**) from Nov 12, 2018.
9. Member of the **Indian Society of Chemists and Biologists (ISCB)** (Membership Fellow Number: **LF-882/18**) from July 9, 2018.
10. Member of the **American Chemical Society (ACS)** (Membership Number: **31022128**) since 2017.
11. Member of the **Association of Chemistry Teachers (ACT)** (Membership No: **1772**) from Nov 23, 2015.

Offline-Online Conference/Workshop/Seminar/Webinar Organized (3)

1. Role as a Co-convenor for the "E-Summit 2024" organized by E-Cell, ROLTA Centre, MANIT Bhopal.
2. Role as a **Convenor** in an "Online Webinar Series 2023" on "Blending of Forensic Science with Law - Crime Spot to Court Room" organized by **Department of Chemistry** and 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 PàvlosG. Kipouràs, Judicial and Professional Graphologist, *University of Thrace, Greece*).

3. Role as a **Convenor** in an “Online Webinar Series 2023” on "Blending of Forensic Science with Law - Crime Spot to Court Room” organized by **Department of Chemistry** and 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 Center, Italy*).

Professional Academic Activities (30)

1. Reviewed a research article for **J. Mol. Liq.** (Elsevier) in June **2024**.
2. Reviewed a research article for **ACS Omega** (ACS) in May **2024**.
3. Reviewed a research article in **Computational and Theoretical Chemistry** (Elsevier) in Apr **2024**.
4. Reviewed four research articles for **Frontiers in Chemistry** (Theoretical and Computational Chemistry) in Nov 2021, Feb 2022, April 2022, and July 2022.
5. Reviewed four research articles for **Main Group Chemistry** in Oct **2015**, May **2018**, and July **2021**, April **2022**, and July 2022.
6. Reviewed a research article for **Journal of Cluster Science** (Springer-Nature) in Aug **2017**.
7. Reviewed a research article for **Australian Journal of Chemistry** (CSIRO) in Dec **2017**.
8. Reviewed a research article for **Chemistry Select** (Wiley) in **2018**.
9. Reviewed five research articles for the **Current Computer-Aided Drug Design (CC-ADD)** (Bentham Science) in Jan **2019**, Mar **2019**, Sep **2019**, Jan **2020**, Mar **2020**.
10. Reviewed a research article for the **International Journal of Computational and Theoretical Chemistry** in Feb **2019**.
11. Reviewed a research article for the **Journal of Dispersion Science and Technology** (Elsevier) in Mar 2020.
12. Reviewed four research articles for the **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** in May **2019**, Aug **2020**, Aug **2021**, and June 2023, respectively.
13. Reviewed two research articles for the **Current Pharmaceutical Biotechnology (CPB)** in Aug **2020**.
14. Reviewed a research article for the **Ind. J. Chem** (Elsevier) in May **2020**.
15. Reviewed a research article for the **Chiang Mai Journal of Science** (Elsevier) in Jan **2020**.
16. Reviewed a communication paper for the **Chem. Phys. Lett.** (Elsevier) in Sep **2020**.

Extra-Curricular Activities

1. Worked as 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.
2. Worked as **Buddy**, Counseling Service, PG Wing, **IIT Kanpur** during **2016-2017**.
3. Worked as **Mentor**, Counseling Service, PG Wing, **IIT Kanpur** during **2015-2016**.
4. Worked as **Orientation Team Member**, Counseling Service, PG Wing, **IIT Kanpur** during **2014-2015**.
5. Worked as **Orientation Team Member**, Counseling Service, PG Wing, **IIT Kanpur** during **2013-2014**.
6. Worked as **Maintenance Secretary** of the **Hall-7, IIT Kanpur** during **2014-2015**.
7. Worked as **Anti Noise Committee Member** of the **Hall-7, IIT Kanpur** during **2012-2013**.
8. Worked as **Maintenance Committee Member** of the **Hall-7, IIT Kanpur** during **2012-2013**.
9. Worked as **Volunteer** of Hall Day of the **Hall-7, IIT Kanpur** during **2012-2013**.
10. Worked as **Cultural Committee Member** of the **Hall-7, IIT Kanpur** during **2013-2014**.
11. Worked as **Volunteer** of Hall Day of the **Hall-7, IIT Kanpur** during **2013-2014**.
12. Participated in **10 KM MARATHON** and **completed successfully** organized by **Adventure Club, Games and Sports Council, IIT Kanpur** on **Mar 15, 2015**.
13. 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 Institute

1. ERP Coordinator of the Department of Chemistry, MANIT Bhopal.
2. Assistant Warden of Hostel 1 (Homi Jahangir Bhabha Hostel) in MANIT Bhopal.
3. Co-convenor of E-Summit 2024 organized by E-Cell, ROLTA Centre, MANIT Bhopal.
4. Coordinator of "Industry Connect" in the Department of Chemistry, Manipal University Jaipur.
5. Co-coordinator of M.Sc. (Chemistry) Program in the Department of Chemistry, Manipal University Jaipur (2023-2025).
6. Lead role in a Summer Camp organized by the Department of Chemistry, Manipal University Jaipur dated May 11, 2023.
7. Admission Committee Member (B.Sc., M.Sc., and B.Sc. + L.L.B.) for 2023-24 (Manipal University Jaipur)
8. Academic Administration and Mentoring in the Department (Chemistry) and Institute (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*

.....**END**.....