

Dr Ruchi Gaur

Assistant Professor

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Researchgate Id: https://www.researchgate.net/profile/Ruchi_Gaur6

Research Summary

My research experience spans several multidisciplinary domains, including Coordination Chemistry, Supramolecular Chemistry, Self-Assembly, Coordination Polymers, Bioinorganic Chemistry, Protein and Peptide Chemistry, Nanomaterials, Multicomponent Cocrystals, Polymorphism, and Theoretical Calculations. My research interests are focused on applying these multidisciplinary skills to develop innovative solutions for **human health** and **environmental sustainability** challenges.

Education

2013 Ph.D. Inorganic Chemistry, BHU Banaras Hindu University, Varanasi, India.

2005 M. Sc. Chemistry, CSJM University Kanpur, India.
(Special Papers: 1. Bio-Inorganic & Supramolecular Chemistry
2. Organic Synthesis 3. Polymer Chemistry
4. Organotransition metal complexes
5. Medicinal Chemistry)

2003 B. Sc. Chemistry, CSJM University Kanpur, India.

Ph.D. thesis title *“Synthesis, characterization and applications of some metal complexes of chalcones and a bis-flavanol”*

Supervisor: Prof. Lallan Mishra (Distinguish Professor, Department of Chemistry, Institute of Sciences, BHU Varanasi U P India)

WORK EXPERIENCE

- **Research Scientist** (1st May 2023 – 30th April 2025) SciTech products & DrChem Lab Thane Mumbai-421503 India.

- **Freelance consultant and scientific writer** (2023-2025).
- **Senior Executive-R&D** (12th December 2022 – 17th April 2023) Survival Technologies Ltd. Mumbai-400013 India.
- **Dr. D S Kothari Fellow** (21 November 2019 – 20 November 2022) (with Prof. Gautam R Desiraju) Department of Solid State and Structural Chemistry Unit (SSCU) Indian Institute of Science, Bangalore 560012.

➤ **Start up research grant**

- (1 September 2015- 31st August 2018) **SERB Young -Scientist (SERB (DST)** Sanctioned startup grant (**PI**).
(With Prof. Sandeep Verma, Department of Chemistry, IIT Kanpur UP India)

✚ **Post- Doctoral work**

- (2nd April 2014 -31st August 2015) *"Inhibition of Insulin by Small Molecules"*
(Supervisor: Prof. Sandeep Verma, Department of Chemistry, IIT Kanpur)

- (24th Feb 2013- 31st March 2014) *"Development of novel metal-organic frameworks for recognition studies"*
(Supervisor: Prof. Lallan Mishra, Department of Chemistry, BHU UP India)

✚ **Pre-Doctoral work**

- (19th January 2008- 31st January 2009) *"Synthesis and cellular & molecular Bioassay of Cytotoxic Ru-complexes as Anti-cancer Agent"*
(Supervisor: Prof. Lallan Mishra, Department of Chemistry, BHU Varanasi U P India
Co-Supervisor: Prof. S. K. Trigun Department of Zoology BHU Varanasi U P India)

Achievement and award

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|------------------------|--|
| 2005 | Vocational Training Certificate "Solving Challenges of Chemistry through Analysis" From IIT Kanpur with II nd position. |
| 2006 & 2007 | Qualified CSIR -National Eligibility Test (CSIR-NET) India held in NET (LS) |
| 2007 | Graduate Aptitude Test in Engineering "GATE -2007". |
| 2009 | Award of UGC Research Fellowship |
| 2013 | SERB (DST) Sanctioned startup research grant (SERB young scientist) |
| 2019 | Award of women scientist scheme C 2019 on IPR (One month orientation and two months hands on training in Law Firm 2019. |

(Intellectual Property Right and Management of Patent System)

2019

Award of DS Kothari Fellowship 2019.

Sponsored Research Project

- ✚ SERB (DST) Sanctioned startup research grant (SERB young scientist) project entitled "***Tuning of adenine based receptors for recognition studies***" about 30.5 Lakhs from 1st September 2015 to 31st August 2018.
- ✚ UGC Sponsored D S KOTHARI research grant project entitled "***Development of modulated photoinduced molecular crystals for photoresponsive objects***" about 26.5 Lakhs from 21st November 2019 to 20th November 2022.

Teaching Experience

Assisted B. Sc. General Chemistry course as lab tutor for two semesters in Department of Chemistry, BHU, India (2012-2013).

Technical Skills

1. Excellent experience in conducting reactions under inert conditions.
2. Purification, and characterization of various organic and inorganic compounds in milligram and multigram scale.
3. *Handling Air-free Techniques:* Glove box, Schlenk lines.
4. *Chromatographic Techniques:* Column, Flash, Paper and Ion-exchange chromatography, HPLC.
5. *Analytical Characterization Techniques:* Multinuclear NMR, EPR, IR, Mass Spectrometry (FAB-MS and ESI-MS), CHN analysis, UV-Vis spectroscopy, Fluorescence spectroscopy, Circular Dichroism, Cyclic Voltammetry.
6. *Crystallographic Techniques:* Crystal growing methods, Single-crystal X-ray diffraction, Crystal solving (WinGx, SHELXTL, PLATON, Olex) and visualizing (Diamond, Mercury, ORTEP) software, Crystal explorer for hirshfeld surface analyses, ToposPro (Topology determination).
7. *Materials fabrication and characterization Techniques:* Hydrothermal technique, TGA, Optical microscopy, SEM, AFM, TEM.
8. *Biophysical Techniques:* Isothermal titration calorimeter, Gel electrophoresis.
9. *Computational Program:* DFT calculations for small organic and inorganic molecules using Gaussian 09/16 programs, Autodock (Molecular docking), Molecular docking visualization (Pymole, Discovery studio), Gaussview6, Multiwfn.

RESEARCH CONTRIBUTION

Total number = 30

h-index = 13

Publications

1. **Ruchi Gaur***, Unraveling non-covalent interactions in bis-chalcone: A crystallographic and theoretical studies *Journal of Molecular Structure* 1297 (2024) 136952 (ISSN: 0022-2860, Impact Factor: 4.7)
2. **Ruchi Gaur***, Sourav Roy, Subhasis Samai, Scope and design of diversified supramolecular synthons of 5-hydroxyisophthalic acid: Crystallographic and theoretical investigations *Journal of Molecular Structure* 1321 (2025) 140097 (ISSN: 0022-2860, Impact Factor: 4.7)
3. Rosidah Sunaiwi, **Ruchi Gaur**, Mohammad Khairul Azhar Abdul Razab, Fara Hana Hadzuan, Norazlina Mat Nawati, Mohd Zahri Abdul Aziz, Anam Mohamed Noor, Nur Atiqah Syahirah Shari, Zulhisyam Abdul Kari, Ajay Guru, Parashuram Kallem, Synthetic and natural antibacterial carbon adsorbents for clinical nuclear waste management *Heliyon* 10 (2024) e38682 (ISSN: 2405-8440, Impact Factor: 3.6)
4. **Ruchi Gaur***, Polymorphism in parabanic acid-urea cocrystals governed by Supramolecular Synthons: A comparative analysis *CrystEngComm*, 25 (2023) 4680-4689 (ISSN: 1466-8033, Impact Factor: 2.6).
5. **Ruchi Gaur***, Combined experimental and theoretical studies of bis-chalcone: Estimation of non-covalent interactions *Journal of Molecular Structure* 1282 (2023) 135189-135198 (ISSN: 0022-2860, Impact Factor: 4.7)
6. **Ruchi Gaur***, Lallan Mishra* Supramolecular and theoretical investigation of copper(II) complexes containing 2,2'-bipyridine and substituted chalcone ligands: Estimation of non-covalent interactions *Journal of Molecular Structure* 1273 (2023) 134271 (ISSN: 0022-2860 Impact Factor: 4.7).
7. **Ruchi Gaur***, Sourav Roy+, Mithun Paul+, Madhu Rajkumar+, and Gautam R. Desiraju* Synthetic strategies towards higher cocrystals of some resorcinols *Crystal growth and design* 22 (12) (2022) 7578–7589. (ISSN: 1528-7483, Impact Factor: 4).
8. **Ruchi Gaur***, Parashuram Kallem Structural and theoretical study of copper(II) complex incorporating chalcone and 2,2'-bipyridine mixed ligands : A probable candidate for optical material *New J. Chem.*, 46 (2022) 20366–20376 (ISSN: 1369-9261 Impact Factor: 2.5).
9. **Ruchi Gaur***, Sourav Roy, Parashuram Kallem, Fawzi Banat, Experimental and theoretical investigation of hydrogen bonded supramolecular assemblies through water

- molecules in a copper(II)-EGTA complex *Journal of Molecular Structure* 1265 (2022) 13340-13350 (ISSN: 0022-2860 Impact Factor: 4.7).
10. Parashuram Kallem*, Ravi P. Pandey, Hanaa M. Hegab, **Ruchi Gaur**, Shadi W. Hasan, Fawzi Banat High-performance thin-film composite forward osmosis membranes with hydrophilic PDA@TiO₂ nanocomposite substrate for the treatment of oily wastewater under PRO mode. *J Environ. Chem. Eng.* 10 (2022) 107454 (ISSN NO. 22133437, Impact Factor: 7.2).
 11. Parashuram Kallem*, **Ruchi Gaur**, Ravi P. Pandey, Shadi W. Hasan, Heechul Choi*, Fawzi Banat*. Thin film composite forward osmosis membranes based on thermally treated PAN hydrophilized PVDF electrospun nanofiber substrates for improved performance. *J. Environ. Chem. Eng.* 9 (2021) 106240 (ISSN NO. 22133437, Impact Factor: 7.2).
 12. **Ruchi Gaur**[†], Priyanka Choudhary[†], Darsi Rambabu, Abhimanew Dhir, Ankush Gupta,* and Pooja* Copper Metallogel as Potential Drug Carrier for Anti-Inflammatory Drugs. *ChemistrySelect* 6 (2021) 9139-9143 (ISSN NO. 2365-6549, Impact Factor: 2).
 13. **Ruchi Gaur*** Ionic nature of cadmium polymer plays decisive role in selective dye adsorption; *Journal of Solid State Chemistry* 278 (2019) 120907 (ISSN NO. 0022-4596, Impact Factor: 3.5).
 14. **Ruchi Gaur*** Selective anionic dye adsorption, Topology and Luminescence study of structurally diverse cadmium(II) coordination polymers. *Inorganic Chemistry Frontiers* 6 (2019) 278–286 (ISSN NO. 2052-1553, Impact Factor: 6.4).
 15. **Ruchi Gaur***, Mohammad Usman, A combined experimental and theoretical investigation of ruthenium(II)-hydrazone complex with double stranded DNA: spectroscopic, molecular docking, nuclease properties and topoisomerase inhibition. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 209 (2019) 100–108 (ISSN NO. 1386-1425, Impact Factor: 4.6).
 16. **Ruchi Gaur**, Diksha Kumari Choubey, Mohammad Usman, Benzamin D. Ward, Jagat Kumar Roy, Lallan Mishra* Synthesis, structures, nuclease activity, cytotoxicity, DFT and molecular docking studies of two nitrate bridged homodinuclear (Cu-Cu, Zn-Zn) complexes containing 2,2'-bipyridine and a chalcone derivative. *J. Photochem. Photobiol. B* 173 (2017) 650–660 (ISSN NO. 1011-1344, Impact Factor: 5.4).
 17. Katarina K. Jovanovic, Nevenka Gligorijevic, **Ruchi Gaur**, Lallan Mishra, Sinisa Radulovic* Anticancer activity of two ruthenium(II)-DMSO-chalcone complexes: Comparison of cytotoxic, pro-apoptotic and antimetastatic potential. *JBUON* 21(2), (2016) 482-490 (ISSN NO. 1107-0625, Impact Factor: 2.533).
 18. **Ruchi Gaur**, Lallan Mishra*, M. Aslam Siddiqi and Burak Atakan* Ruthenium complexes

- as precursor of Chemical Vapour-Deposition (CVD). *RSC Adv.*, 4 (2014) 33785–33805 (**Review Article**) (ISSN NO. 2046-2069, Impact Factor: 4.6).
19. **Ruchi Gaur**, A. L. Susmitha, K. V. R. Chary and Lallan Mishra* Water soluble Calcium-Sodium based coordination polymer: Selective Release of Calcium at Specific Binding Sites on Protein *RSC Adv.*, 4 (2014) 24038–24041 (ISSN NO. 2046-2069, Impact Factor: 4.6).
 20. S. K. Singh, **Ruchi Gaur**, A. Kumar, R. Fatima, Lallan Mishra, and Saripella Srikrishna* The Flavonoid Derivative 2-(4'-Benzyloxyphenyl)-3-hydroxychromen-4-one Protects Against Ab42-Induced Neurodegeneration in Transgenic Drosophila: Insights from In Silico and In Vivo Studies. *Neurotox. Res.* 26 (2014) 331–350 (ISSN NO. 1476-3524, Impact Factor: 3.3).
 21. **Ruchi Gaur** and Lallan Mishra* Bi-nuclear Ru(II) complexes of bis-chalcone and bis-flavonol: synthesis, characterization, photo cleavage of DNA and Topoisomerase I inhibition. *RSC Adv.* 3 (2013) 12210–12219 (ISSN NO. 2046-2069, Impact Factor: 4.6).
 22. **Ruchi Gaur** and Lallan Mishra* Synthesis and Characterization of Ru(II)–DMSO–Cl–Chalcone Complexes: DNA Binding, Nuclease, and Topoisomerase II Inhibitory Activity. *Inorg. Chem.* 51 (2012) 3059–3070 (ISSN NO. 0020-1669, Impact Factor: 4.7).
 23. **Ruchi Gaur**, R. A. Khan, S. Tabassum, P. Shah, M. I. Siddiqi, Lallan Mishra* Interaction of a ruthenium(II)–chalcone complex with double stranded DNA: Spectroscopic, molecular docking and nuclease properties. *J. Photochem. Photobiol., A* 220 (2011) 145–152 (ISSN NO. 1010-6030, Impact Factor : 4.7).
 24. R. Prajapati, S. K. Dubey, **Ruchi Gaur**, R. K. Koiri, B. K. Maurya, S. K. Trigun, Lallan Mishra* Structural characterization and cytotoxicity studies of ruthenium(II)–dmschloro complexes of chalcone and flavone derivatives *Polyhedron* 29 (2010) 1055-1061 (ISSN NO. 0277-5387, Impact Factor: 2.6).

Book Chapters

1. Environmental impacts and life cycle analysis of green nanomaterials.
Ruchi Gaur*,
Green Functionalized Nanomaterials for Environmental Applications, Edited by: Uma Shanker, Chaudhery Mustansar Hussain and Manviri Rani **Elsevier Publication**, 2021, 511-540. (ISSN NO. 9780128231371)
2. Rational insight approaches of environmental remediation through metal green

- nanomaterials. **Ruchi Gaur***, Parashuram Kallem , Dipankar Sutradhar*, Fawzi Banat Handbook of Green and Sustainable Nanotechnology, edited by Uma Shanker, Chaudhery Mustansar Hussain and Manviri Rani **Springer Publication** 2022. 1-35 (ISSN NO. 9783030690236)
3. Application of Nanoclusters in Environmental and Biological Fields: Experimental and Theoretical Approaches.
Dipankar Sutradhar*, Sourav Roy and **Ruchi Gaur***, Handbook of Green and Sustainable Nanotechnology, edited by Uma Shanker, Chaudhery Mustansar Hussain and Manviri Rani, **Springer Publication** 2022, 1-21. (ISSN NO. 9783030690236)
4. Tuning of Ruthenium-DMSO Complexes for a search of new anticancer agent
Ruchi Gaur*, Lallan Mishra Ruthenium Chemistry Book, **Pan Stanford Publisher**, Singapore 2017, PAGE NO 337-375. <https://doi.org/10.1201/9781315110585> (ISSN NO. 978-981-4774-39-0)
5. Diffusion and Transport of Molecules In Living Cells
Ruchi Gaur, Lallan Mishra and Susanta K. Sen Gupta* Modelling and Simulation of Diffusive Processes, Simulation Foundations, Methods and Applications S. K. Basu, Naveen Kumar (eds.), DOI 10.1007/978-3-319-05657-9 © **Springer International Publishing, Switzerland** 2014 page no.27-49(ISSN NO. 2195-2817)
6. TRANSITION METAL COMPLEXES AND THEIR BINDING WITH DNA
N. Kumari, N. Dixit, **R. Gaur**, P. Sinha and L. Mishra* New Trends in Coordination, Bioinorganic, and Applied Inorganic Chemistry Edited by M. Melník, P. Segl'a, M. Tatarko, **Slovak University of Technology Press, Bratislava** © 2011 page no. 320-334 (ISSN NO. 1335-308X)

Conferences & Workshops

- (26-28th December 2008) Oral presentation in 27th Annual conference of Indian council of chemist held in Haridwar.
- (08-09th March 2010) National Symposium-cum-Workshop on X-Ray Crystallography" Department of Chemistry, BHU Varanasi-221005.
- (11-13thDecember2010) Poster Presentation in the International symposium on Frontiers in Inorganic Chemistry (FIC-2010) held in IACS Kolkata.
- (19-20th February2011) Emerging trends in Chemical sciences (ETCS-2011) held in BHU Varanasi.

- (14-15th June 2011)** Oral presentation in 13th International conference of the International Academy of Physical Sciences (CONIAPS-XIII) held in University of Petroleum and energy studies, Dehradun.
- (3-7th December 2011)** Oral presentation in 48th annual convention of chemists 2011 (Indian chemical Society) held in Allahabad University, Allahabad.
- (3-5th February 2012)** Poster presentation in 14th CRSI National symposium in Chemistry held at National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram.
- (31st Jan-3th February 2013)** Poster presentation in 3rd RSC meeting and 15th CRSI National symposium in Chemistry held at Banaras Hindu University, Varanasi.
- (6 – 8th November 2017)** Poster presentation in UK-India Newton Researcher Links Workshop on Peptides, Proteins and Metals in Disease and Therapy Indian Institute of Technology Kanpur, India.
- (11-14th December 2017)** Poster presentation in Modern Trends in Inorganic Chemistry (MTIC) in NCL and IISER Pune, India.
- (17-21, November 2020)** Short Term Course on Nanomaterials for Environmental Applications: Characterization by Analytical Tools in Department of Chemistry, MNIT Jaipur & NIT, Jalandhar India.
- (16th, September 2021)** AWSAR (Augmenting writing skill for Articulating research skill) webinar on popular science writing organized by DST India and Vigyan Prasar (VP).
- (22-23rd, September 2021)** RSCIISER Desktop seminar with CrystEngComm
- (14th, October 2021)** AWSAR (Augmenting writing skill for Articulating research)
- (27-28th, October 2021)** RSCIISER Desktop seminar with JMC-A.

Other Activity

Life Time member of Chemical Research Society (CRSI) of India, Bangalore, India

Reviewer of Journals

Inorganic Chemistry (ACS), RSC Advances, Applied Organometallic Chemistry, Journal of Applied Polymer Science; Journal of Environmental Chemical Engineering, Chemosphere, Journal of Molecular Structure, Chemistry Select, Spectrochem. acta A, Material sciences in semiconductor processing, Inorganic chemistry communication, Energy nexus, Archives of biochemistry and biophysics, ACS Omega, Journal of inorganic and general chemistry (Wiley)