Dr. Azaj Ansari
Assistant professor
Department of Chemistry,
Central University of Haryana,
Jant-Pali, Mahendergarh - 123031
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Educational Qualifications:

- Doctor of Philosophy (**Ph.D** - March 2016), Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India.
- Master of Science **(M.Sc**), Department of Chemistry, Jamshedpur Co-operative College, Ranchi University, Ranchi, India.

Visiting Theoretical Scientist:

February - April 2015, Prof. Peter Comba's Lab, Institute of Inorganic Chemistry, University of Heidelberg, Germany.

Awards and Distinction:

- Qualified Graduate Aptitude Test in Engineering (GATE) 2011.
- Qualified Council of Scientific & Industrial Research (CSIR)-JRF 2011.
- Junior and Senior Research Fellowship, January 2011-June 2016.
- **Best Oral Presentation Award in** the National Symposium on Current Trends in Chemical and Nano Sciences (*CTCNS-2014*)", Shivaji University, Kolhapur, India, 17^{th}-18^{th} January 2014.
- **Best Oral Presentation Award in** the "Catalysis Scholars Meet 2014 *(CATSCHOL 2014*)", Institute of Chemical Technology, Mumbai, India, ^{4th} March 2014.
- **Best Poster Presentation Award in** the *"Chemical Frontiers 2014 (CF2014*)", at Majorda Resort, Goa, India, 6^{th}-9^{th} August 2014.
- **Associate Member of Royal Society of Chemistry** (**AMRSC**) for the year 2014-2015.
- **Society of Biological Inorganic Chemistry (SBIC)** Student Member for the year 2014.
- International conference grant awarded by **IIT Bombay**, 2013.
- International conference grant awarded by **Department of Biotechnology**, Delhi, India, 2014.
- 2^{nd} MCBR Winter School 2015 grant awarded by **University of Heidelberg**, Germany, 2015.

Additional Charge at Central University of Haryana:

- Liaison officer
- Assistant proctor
- Minority representative in teacher's grievance redressal committee
- Member, central admission advisory committee
- Member, standing committee for admissions
- Member, DRC, Department of Chemistry
- Member, RAC, Department of Chemistry

Research Interests:

To employ state-of-the-art of applied computational methods:

- To understand the electronic structures, energetic formations and magnetic properties of inorganic complexes
- To calculate and predict the spectroscopic properties such as EPR, UV-Visible spectra and Mossbauer of Inorganic complexes.
- To understand the reaction mechanism involving regio-selective hydroxylation, epoxidation, C-H bond activation and proton coupled electron transfer reactions of high-valent metal complexes.
- Modelling bio-inspired catalytic reactions - implications to metalloenzymes and model complexes.
- Modelling spin state dependent catalytic reactivity of heme and non-heme iron systems
- To understand the mechanism of energy transfer in photoredox catalysis and its application in water splitting

Our innovative application of the theoretical methods in the field of computational chemistry can lead a design of synthetic mimics by experimental scientist.

List of Project:

Project titled "***Understanding Mechanism of Energy Transfer in Photoredox Catalyst and Its Applications in Catalytic Transformation Reactions***" (Rs. 4089000/-; Completed).

List of Project Assistant

Mr. Manjeet Kumar: Project titled "*Understanding Mechanism of Energy Transfer in Photoredox Catalyst and Its Applications in Catalytic Transformation Reactions*" (**Rs. 4089000**/-; Completed).

List of Ph.D. Students (Ongoing):

1. **Ms. Monika (July 2017):** Project titled "Density Functional Theory Approach towards Electronic Structures, Formation of High-Valent Metal Species and Metal Mediated C-H/O-H Bond Activation" (Thesis submitted on 21-01-2022).

2. **Ms. Oval Yadav (July 2018):** Project titled "Computational Studies on Structures of Metal Complexes and Metal Mediated Catalytic Reactions" (Thesis submitted on 23-06-2022).

3. **Mr. Manjeet Kumar (July 2019):** Project titled "Computational Studies on Structures, Spectroscopic Properties and Role of Transition Metal Complexes in Catalytic Reactions".

4. **Mr. Mukhtar Ahmed (November 2020)**: Project titled "Mechanistic Investigations of Catalytic Transformation Reactions using Transition Metal Complexes: A Computational Exploration".

List of M.Sc. Project Students (Completed):

1. Dissertation title "*A Brief Introduction to Computational Chemistry"* by Mr. Amit Kumar.
2. Dissertation title *"A Computational Approach on High-valent Non-heme Iron-oxo Complexes"* by Ms. Manisha Kumari.
3. Dissertation title *"Computational studies of characterization of iron-oxo compound"* by Mr. Navneet Sharma.
4. Dissertation title "*High-valent Non-heme Iron-oxo Species in Catalytic Reactivity Towards C-H Bond Activation: A Computational Approach*" by Mr. Mandeep Panwar.

5. Dissertation title "*Spectroscopic Characterization of High Valent Iron(III/IV)-oxo Complexes*" by Ms. Sunita Kumari.
6. Dissertation title "*A Computational Approach Towards C-H Activation*" by Mr. Rahul Kumar.
7. Under-graduate project: dissertation title "*Metal Mediated Catalytic Transformation Reaction: A DFT Exploration*" by Mr. Vipin Yadav.
8. Dissertation title "*Electronic Structures of Mechanistic Study of Metal Mediated Catalytic Reactions by [(Mn^{II}(N_3Py_2(H_2O)] Complexes"* by Ms. Trishtha.
9. Dissertation title *"A Computational Approach Towards Oxygenation of Cyclohexene by Nonheme Iron Complex"* by Ms. Hemlata.
10. Dissertation title *"A DFT Exploration on Iron(IV)-oxo Complexes with Protons"* by Mr. Rahul Yadav.
11. Dissertation title "*Electronic Structure and Reactivity of Cobalt Complexes*" by Mr. Bhanu Pratap.
12. Dissertation title "*A Computational Approach on Oxowall of First Transition Series with BUEA Ligand"* by Mr. Aman
13. Dissertation title "*Oxidation of Styrene by Bio-Inspired Non-Heme Iron Complex: A Computational Approach*" by Ms. Kumari Sunita
14. Dissertation title "*A Theoretical Study on Metal Porphyrin N-Heterocyclic Carbenes*" by Ms. Roopa Yadav
15. Dissertation title "*A Computational Approach on Oxowall of First Transition Series with TMC Ligand"* by Ms. Somi
16. Dissertation title "*A Computational Study For Conversion Of CO_2 into CH_4 by A Dinuclear Nickel Catalyst"* by Ms. Isha Yadav
17. Dissertation title "*Role of Basicity of Metal Complexes on C-H Bond Activation: A Computational Exploration*" by Khadim Hussain
18. Dissertation title "*Photooxidation of Aromatic Aldehydes in Presence of Palladium(II) Porphyrin Catalyst*" by Ms. Chanchal Dahiya
19. Dissertation title "*A DFT Study of Pyridine-Based Manganese(III) and Iron(III) Complexes as Superoxide Dismutase Mimics*" by Ms. Anjali Sharma
20. Dissertation title "*Theoretical Study of Fluorecein Based Copper Complexes" by Ms. Bhavna*
21. *Dissertation title*"A Computational Approach on a Novel Di-Carbazole Based Dye" by Mr. Dushyant
22. Dissertation title "*Molecular Docking on Copper (II) Complexes Containing α - Aminophosphonates*" by Ms. Himanshi Mittal
23. Dissertation title "*Natural Bond Orbital Analysis and Electrostatic Potential Map of Alpha Aminophosphonate Ligated Copper Complexes*" by Ms. Kiran Yadav
24. Dissertation title "*A Computational Study of Tris(2-(1H-pyrazol-1-yl)Pyridine Containing Cobalt Species*" by Ms. Kuldeep Yadav
25. Dissertation title "*Spiro-OMETAD Molecule: A Computational Exploration*" by Ms. Shital Yadav
26. Dissertation title "Computational Exploration on Photophysical Properties of Boron Nitride Compounds" by Ms. Anagha K T
27. Dissertation title "Oxidation of Methane by High Valent Iron-oxo with TAML Species: A Comparative Study" by Mr. Ankush Kumar

28. Dissertation title "DFT Study on Dipicolinic Acid and Its Metal Complexes and Molecular Docking Study as New Inhibitor of NDM
29. Dissertation title "Theoretical Explorations of Metal Mediated Intermediates Used for NH3 Oxidation Catalysis" by Ms. Neha
30. Dissertation title "Computational Study on Coumarin Derivatives" by Mr. Yasveer Singh

List of Publications:

1. *"Mechanistic Insights On the ortho-hydroxylation of Aromatic Compounds by Non-heme Iron Complex: A Computational Case Study on the Comparative Oxidative Ability of Ferric-hydroperoxo and High-valent $Fe^{IV}=O$ and $Fe^{V}=O$ Intermediates"* **Azaj Ansari**, Abhishek Kaushik and Gopalan Rajaraman, *J. Am. Chem. Soc.* **2013**, *135*, 4235.

2. *"Theoretical Studies on Concerted versus Two Steps Hydrogen Atom Transfer Reaction by a non-heme $Mn^{IV/III}=O$ complexes: How Important is the Oxo Ligand Basicity in the C-H Activation Step"* Madhavan Jaccob, **Azaj Ansari**, Bhawana Pandey and Gopalan Rajaraman, *Dalton Trans*. **2013**, *42*, 16518.

3. *"Ortho- Hydroxylation of Aromatic Acids by a non-heme $Fe^{V}=O$ species: How important is the ligand design?"* **Azaj Ansari** and Gopalan Rajaraman, *Phys. Chem. Chem. Phys.* **2014**, *16*, 14601.

4. *"Data Set for Modelling Reaction Mechanisms Using Density Functional Theory: Mechanism of ortho-hydroxylation by High-valent Iron-oxo Species"* **Azaj Ansari** and Gopalan Rajaraman, *Dataset Papers in Science*, **2014**, *2014*, 1.

5. *"C-H Bond Activation by Metal-Superoxo Species: What Drives High Reactivity"* **Azaj Ansari**, Prabha Jayapal and Gopalan Rajaraman, *Angew. Chem. Int. Ed.* **2015**, *54*, 564.

6. *"Structures, Bonding and Reactivity of Fe and Mn High-valent Metal-oxo Complexes: A Computational Examination"* Bhawana Pandey, **Azaj Ansari**, Nidhi Vyas and Gopalan Rajaraman, *J. Chem. Sci*. **2015**, *127*, 343.

7. *"Oxidation of Methane by an N-bridged High-Valent diiron-oxo Species: Electronic Structure Implications to the Reactivity"* Mursaleem Ansari, Nidhi Vyas, **Azaj Ansari**, and Gopalan Rajaraman, *Dalton Trans*. **2015**, *44*, 15232-15243.

8. "*Computational Examination on the Active Site Structure of (peroxo)diiron(III) intermediate in the Amine oxygenase, AurF*" Prabha Jayapal, **Azaj Ansari** and Gopalan Rajaraman, *Inorg. Chem.* **2015**, *54*, 11077.

Publications after joining at Central University of Haryana

9. *"Interplay of Electronic Cooperativity and Exchange Coupling in Regulating the Reactivity of Diiron(IV)-oxo Complexes Towards C-H and O-H Bond Activation"*, **Azaj Ansari**, Mursaleem Ansari, Asmita Singha, Gopalan Rajaraman, *Chemistry -A European Journal*, **2017**, *23*, 10110.

10. *"Axial vs. Equatorial Ligand Rivalry in Controlling the Reactivity of Iron(IV)-Oxo Species: Single-State vs. Two-State Reactivity"*, Ravi Kumari, **Azaj Ansari**, Gopalan Rajaraman, *Chemistry -A European Journal*, **2018**, *24*, 6818.

11. *"A Combined Experimental and Theoretical Approach to Structure, Magnetic Properties and DNA Binding Affinity of a Homodinuclear Cu(II) Complex"*, M. N. Ahamad, M. Shahid, **A. Ansari**, M. Kumar, I. M. Khan, M. Ahmad, Rahisuddin, R. Arif, New Journal of Chemistry, **2019**, *43* 7511-7519.

12. *"Unprecedented isolation of a dinuclear tin(II) complex stabilized by pyridine-2,6-dimethanol: structure, DFTand in vitro screening of cytotoxic properties"*, I. Mantasha, M. K. Raza, M. Shahid, **A. Ansari**, M. Ahmad, I. M. Khan, Applied Organometallic Chemistry, **2019**, *33*, 1-8.

13. *"Synthesis, Characterization, Theoretical Studies and Catecholase Like Activities of [MO6] Type Complexes"*, M. Naqi Ahamad, M. Kumar, **A. Ansari**, I. Mantasha, M. Ahmad, M. Shahid, New Journal of Chemistry, **2019**, *43*, 14074-14083.

14. *"Exploring Solvent Dependent Catecholase Activity in Transition Metal Complexes: An Experimental and Theoretical Approach"*, I. Mantasha, M. Shahid, **A. Ansari**, M. Kumar, M. N. Akhtar, M. A. AlDamend, Y. Somge, M. Ahmad, I. M. Khan, New Journal of Chemistry, **2020**,***44***, 1371-1388.

15. *"Anticancer Properties, Apoptosis and Catecholase Mimic Activities of Dinuclear Cobalt(II) and Copper(II) Schiff Base Complexes"*, M. Naqi Ahamad, K. Iman, M. K. Raza, M. kumar, **A. Ansari,** M. Ahmad, M. Shahid, Bioorganic Chemistry, **2020**, *95*, 103561.

16. *"Exploring Catecholase Activity in Dinuclear Mn(II) and Cu(II) Complexes: An Experimental and Theoretical Approach"*, M. S. Ahmad , M. Khalid, M. S. Khan, M. Shahid , M. Ahmad, Monika, **A. Ansari,** M. Ashafaq, New Journal of Chemistry, **2020**, ***44***, 7998-8009.

17. *"Mechanistic Insights of Allylic Oxidation of Aliphatic Compound by Tetraamido Iron(V) Species: A C-H vs. O-H Bond Activation"*, Monika, **A. Ansari**[*], New Journal of Chemistry, **2020**, *44*, 19103-19112.

18. "*Electronic structures, bonding and spin state energetics of biomimetic mononuclear and bridged dinuclear iron complexes: A computational examination*", Monika, Oval Yadav and Hemlata and **A. Ansari**[*]**,** Structural Chemistry, 2020, *32*, 1473-1489.

19. "*An efficient synthesis towards the core of Crinipellin: TD-DFT and docking studies*", Raghaba Sahu, Ranjan K. Mohapatra, Saud I. Al-Resayes, Debadutta Das, Pankaj K. Parhi, Shakilur Rahman, Lucia Pintilie, Manjeet Kumar, Mohammad Azam, **Azaj Ansari***, Journal of Saudi Chemical Society, 2021, 25, 101193.

20. "*A side-on Mn(III)-peroxo supported by a Non-heme Pentadentate N_3Py_2 ligand: synthesis, characterization and Reactivity Studies***,** Dattaprasad. D. Narulkar, **Azaj Ansari**, Anil Kumar Vardhaman, Sarvesh S. Harmalkar, Giribabu Lingamallu, Vishal M. Dhavale, Muniyandi

Sankaralingam, Sandip Das, Pankaj Kumar, Suner N. Dhuri, **Dalton Transactions**, 2021, 50, 2824-2831.

21. *"Electronic structures, bonding and energetics of non-heme mono and dinuclear iron-TPA complexes: a computational exploration"*, O. Yadav, M. Ansari, **Azaj Ansari*** Structural Chemistry 2021, 32, 2007-2018.

22. "*How to identify a smoker: A salient crystallographic approach to detect thiocyanate content*", Khushboo Iman, M. Naqi Ahamad, Monika, **Azaj Ansari,** Hatem A. M. Saleh, M. Shahnawaz Khan, Musheer Ahmad, Rosenani A. Haque, M. Shahid RSC. Advances, 2021, 11, 16881-16891.

23. "*Structure, DFT studies and evaluation of catechol oxidase (CO) mimic activity of mononuclear Co(II) complexes derived from aminoalcohols: An experimental and theoretical approach*", Mantasha I, Mohd Zeeshan, Oval Yadav, **Azaj Ansari**, Khalil M. A. Qasem, Muhammad Nadeem Akhtar, Murad A. AlDamen, M. Shahid, Journal of Biomolecular Structure & Dynamics, 2021.

24. *Elucidating the contribution of solvent on the catecholase activity in a mononuclear Cu(II) system: an experimental and theoretical approach*, M.Shahid, I.Mantasha, Shabnam Khan, Mohd Mehtab, Oval Yadav, **Azaj Ansari**, Khalil M. A. Qasem, Azaz Ahmed, Mariyam Saniya, Muhammad Nadeem Akhtar, Murad A. AlDamen, Journal of Molecular Structure, 2021, 1244, 130878.

25. *Novel {Cu4} and {Cu4Cd6} Clusters Derived from Flexible Aminoalcohols: Synthesis, Characterization, Crystal Structures, and Evaluation of Anticancer Properties*, Khushboo Iman, Md Kausar Raza, Mursaleem Ansari, Monika, **Azaj Ansari**, Musheer Ahmad, M. Naqi Ahamad, Khalil M. A. Qasem, Sameer Hussain, Muhammad Nadeem Akhtar and M. Shahid **Dalton Trans.**, 2021, 54, 11941-11953.

26. "Structural investigations, Hirsfeld surface analyses, and molecular docking studies of a phenoxo-bridged binuclear Zinc(II) complex" M. Azam, P. K. Sahoo, R. K. Mohapatra, M. Kumar, **A. Ansari**,* S. Moon, A. Chutia, S. I. Al-Resayes, S. K. Biswal, Journal of Molecular Structure, **2022**, 1251, 132039.

27. "Effect of Ring Size of TMC Ligands in Controlling C-H Bond Activation by Metal-Superoxo" Monika, **A. Ansari***, Dalton Transactions, **2022**, 51, 5878-5889.

28. "Electronic Structures, Bonding Aspect and Spectroscopic Parameters of Homo/Hetero Valent Bridged Dinculear Transition Metal Complexes" O. Yadav, M. Ansari and **A. Ansari***, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121331 (1-11).

29. "Chemoselective detection based on experimental and theoretical calculations of Cu^{2+} ions via deprotonation of chromone derived probe and its applications" P. Bhalla; N. Tomer; A. Goel; Monika, **A. Ansari** and R. Malhotra, Journal of Molecular Structure, **2022**, 1264, 133251(1-12).

30. "Computational Studies on Potential New Anti-Covid-19 Agents with Multi-Target Modes of Action" R. K. Mohapatra, M. Azam, P. K. Mohapatra, A. K. Sarangi, M. Abdalla, L. Perekhoda, O. Yadav, S. I. Al-Resayes, K. Jong-Doo, K. Dhama, **A. Ansari***, V. Seidel, S. Verma, M. K. Raval, Journal of King Saud University-Science, 202234, 102086 (1-8).

31. "Theoretical Insights for Generation of Terminal Metal-Oxo Species: Drives for "Oxo Wall" "Monika, Aman and **A. Ansari***. New Journal of Chemistry, 2022 (10.1039/D2NJ03098E).

32. "Electronic Structures and Energetic of Metal(II)-Superoxo Species: A DFT Exploration". Monika and **A. Ansari***, Structural Chemistry, 2022.

33. "Electronic, geometrical and photophysical facets of five-coordinated porphyrin N-heterocyclic carbene transition metals complexes: A theoretical study", M. Kumar, M. Ansari and **A. Ansari*,** Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2022.

Invited Talks/Oral Presentations:

1. In International Conference on "*Structural and Physical Properties of Solids* (*SPPS 2013*)", Indian School Of Mines, Dhanbad, India, 18th -20th October 2013. ***"C-H Bond Activation by a Non-heme Iron (V)-oxo Complex: How Strong is this oxidant?"***

2. In the National Synposium on "*Current Trends in Chemical and Nano Sciences* (*CTCNS-2014*)", Shivaji University, Kolhapur, India, 17th-18th January 2014. **"*A Computational Investigation on the ortho-hydroxylation of aromatic Acid by a non-heme Iron Complex"*.**

3. In the National Conference "*Catalysis Scholars Meet 2014 (CATSCHOL 2014)*", Institute of Chemical Technology, Mumbai, India, 4th March 2014. "***Role of High-Valent Metal-oxo Species in Catalytic Reactions: A Detail Computational Study***".

4. In the International Conference "*7th Asian Biological Inorganic Chemistry Conference* (*AsBIC7*)", Crown Plaza, Gold Coast, Australia, 30th November - 5th December 2014. "***A Computational Approach to Understand the Mechanism of α-ketoglutarate Dependent & Related Models*".**

5. In the International Conference "4th Indo-German Seminar on Modeling of Chemical and Biological Reactivity (*MCBR*)", at Indian Institute of Technology, Delhi, India, 7th November 2015. "***Theoretical Study on C-H Bond Activation by High-valent Meta-superoxo Species***".

6. In the International Conference "*American Chemical Society (ACS) on Campus*", at Indian Institute of Technology, Bombay, India, 25th January 2016. "***Role of non-heme Iron(V)-oxo species in C-H Bond Activation"***.

Invited Talks/Oral Presentations after joining at Central University of Haryana

7. In the International Conference *"The international conference on frontier in chemistry (ICFCS-2017)"*, at Applied Chemistry, Central University of Jharkhand, Ranchi, India, 16th-18th March 2017. ***"Role of High-valent Metal-oxo Species in C-H Activation: A Computational Approach"***.

8. In the International Conference *"Industrial Impacts on Environmental and Sustainable Development (IIESD-2018)"*, at Government College of Engineering Keonjhar, Odisha, India, 15th-16th April 2018. ***"Electronic Structure and Mechanistic Study of Biomimetic Catalytic Transformation Reactions: A Computational Approach"***.

As a Resource Person:

1. In the 5 day's Short Term Course on "*Strategies to Enhance Research Visibility, Impact & Citations*" which is scheduled at Government College of Engineering, Keonjhar, Odisha, India from 14th-18th December 2020. **"*Organizing and presenting your research data*".**

2. In 11 days International Workshop on "***Supporting Chemistry Research with modern DFT (Density Functional Theory): Software, Techniques, and Applications*"** Department of Chemistry, Sankalchand Patel University, Gujarat, India, **5th-15th February 2021.**

Extension Lectures:

- ***"Role of High-valent Metal-xo Species in Catalytic Reactions?"*** Government College, Narnaul, Haryana, 4th February 2017.
- ***"Role of Computational Chemistry"*** Chaudhary Bansi Lal University, Bhiwani, 29th April 2019.
- ***"Computational Chemistry"*** Chaudhary Bansi Lal University, Bhiwani, 4th May 2019.
- ***"Basic of Computational Chemistry"*** Indira Ghandhi University, Meerpur, May 2021.

National Conference/ Workshop:

- As an **organizer,** *"**Recent Trends in Eco-Friendly Chemistry (RTEC 2016)**"*, 29th September 2016, Central University of Haryana, Mahendergarh, Haryana.
- As a **Joint Organizing Secretary** "***Intellectual Property Rights: Awareness and Implementaion***", 25th January 2020, Department of Chemistry, Central University of Haryana, Mahendergarh, Haryana.
- As an **Organizing Committee Member,** Event on the theme "**Talk on the theme: Mental Health for All-Greater Investment-Greater Access"** organized by Cell for Person with Disability, Central University of Haryana, Mahendergarh on 2nd October 2020.
- As an Organizing Committee Member**,** Event on the theme **"International Day of Persons With Disabilities"** organized under Cell for Person with Disabilities, Central University of Haryana, Mahendergarh, Haryana on 3rd December 2020.
- As a **Coordinator** in the Webinar on the theme *AZADI KA AMRUT MAHOTSAVA* organized by Department of Management Studies and Cell for Person with Disability, Central University of Haryana, Mahendergarh was held on 18th May, 2021.
- As a **Coordinator** in the National Workshop (Online) "***Hands on Training on RT-PCR Testing Kit and Sanitizers***" on the theme *AZADI KA AMRUT MAHOTSAVA* held organized by the Department of Chemistry, School of Basic Sciences, Central University of Haryana, Mahendergarh, Haryana, India on 29th May, 2021.

UGC UGC Sponsored Orientation/Refresher Courses:

1. Attended in UGC Sponsored four weeks Orientation Course at UGC-HRDC JNU, New Delhi, India, 8th October - 11th November 2018.

2. Attended in UGC Sponsored two weeks Interdisciplinary Refresher Course on Advanced Instrumentation Techniques (Chemical Sciences, Life Sciences, Pharmaceuticals Sciences and Physical Sciences) at UGC-HRDC GJUS&T Hisar, Haryana, India, 11th - 23th November - 11th November 2019.

3. Attended UGC Sponsored two weeks online Refresher Course in Chemistry at UGC-HRDC Punjabi University, Patiala, 29th November - 11th December 2021.

4. Attended UGC Sponsored online two week Interdisciplinary Refresher Course in Advanced Research Methodology, Teaching Learning Centre, Ramanujan College, University of Delhi under the aegis of Ministry of education Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching 22nd July - 05th August 2022.

Conferences, Meetings and Poster Presentations:

1. *"3rd Indo-German Conference",* Indian Institute of Technology, Bombay, Mumbai, India, 27th-29th September 2011.
2. "*3rd Asian Conference on Coordination Chemistry",* New Delhi, India, 17th -20th October 2011.
3. *"International Symposium on Chemistry & Complexity",* Indian Association for the Cultivation of Science Kolkata, India, 6th -8th December 2011.
4. "*IIT Bombay-ACS Symposium*" Indian Institute of Technology, Bombay, Mumbai, India, 2nd October, 2012.
5. *"Theoretical Chemistry Symposium 2012* (*TCS12*)*",* Indian Institute of Technology, Guwahati, India, 19th-22th December 2012**.**
6. "*3rd Indo-German Conference on Modeling Chemical Biological Reactivity (MCBR3)*", NIPER & IISER Mohali, India, 27th February – 1st March 2013.
7. "*Symposium on Theoritical and Computational Chemistry – Frontiers and Challenges* (*STCC-FC*)", Bharathidasan University, Tiruchirappalli, Tamilnadu, India.
8. "*15th International Conference on Density Functional Theory and its Applications* (*DFT 2013*)", Durham University, Durham U.K. 9th -13th September 2013.
9. *"National Symposium on 16th Chemical Research Society of India* (*CRSI*)*",* Indian Institute of Technology Bombay, Mumbai, India, 7th -9th February2014.
10. "*Workshop on Electronic Structure, Atomistic and Statistical Modeling in Chemistry, Materials and Life Science*", Institute of Chemical Technology, Mumbai, India, 5th-7th August 2014.
11. "*Chemical Frontiers 2014* (*CF2014*)", at Majorda Resort, Goa, India, 16th-19th August 2014.
12. *"Theoretical Chemistry Symposium 2014* (*TCS14*)*",* National Chemical Laboratory, Pune, India, 18th-21st December 2014**.**
13. "*Modeling of Chemical and Biological Reactivity* (*2nd MCBR Winter school 2015*)", at University of Heidelberg, Germany, 17th-22nd February 2015.

14. *"4th Indo-German Meeting on Modeling of Chemical and Biological Reactivity (MCBR2015)",* at University of Heidelberg, Germany, 23rd-25th February 2015.

Conferences and Meetings after joining at Central University of Haryana

15. "*Conference on Modern Trends in Molecular Magnets (MTMM)*" organized by department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India, 19th -21th May 2016.
16. *"8th Asia Pacific Conference on Theoretical and Computational Chemistry*", Indian Institute of Technology Bombay, Mumbai, India, 15th -17th December 2017.
17. Three Days National Workshop on "Teaching, Learning and Evaluation Online with Moodle Moocs Platform & Open Education Resources" organized by Department of Education & School of Education, Central University of Haryana, Mahendergarh, 14th - 16th May 2018.
18. A Webinar on "BET Surface Area analysis and Catalyst Characterization" at Central University of Haryana, Mahendergarh, 22th May, 2020.
19. A Webinar on "Nature to Nurture" at Vivek College, Bijnor, UP, 05 June 2020.
20. A National Webinar Series on "Research Methodology" at Loyola College, Chennai, Tamil Nadu, 12th -13th June, 2020.
21. One-Week Online Faculty Development Programme on "Development and Delivery of MOOCs and E-Content" jointly organized by Central University of Haryana, Mahendergarh and Deshbandhu College, University of Delhi, New Delhi, 26th June- 1st July 2020.
22. Deliver a talk on the theme *"***Talk on the theme: Mental Health for All-Greater Investment-Greater Access" organized by** Cell for Person with Disability, Central University of Haryana, Mahendergarh on 2nd October 2020.
23. Participated in a National Webinar on '**Training on Skill Development programme for Atmanirbhar Bharat**' organized by BioMedical Sciences, Department of Vocational Studies & Skill Development, Central University of Haryana on 9th June,2021.
24. Participated in a National Webinar on "**Training on Skill Development Programme for Aatmnirbhar Bharat**" under 'Azadi ka Amrut Mahotsav' organized by Industrial Waste Management, Department of Vocational Studies & Skill Development, Central University of Haryana, Mahendragarh on 10th June, 2021.
25. Participated in a National Webinar on "**Post-Independence Scenario of Renewable Energy Resources in India**" held on June 2, 2021, Organized by Department of Physics & Astrophysics, Central University of Haryana, Mahendergarh-123031.
26. Participated in a School Level Workshop (Online) "**Curricula Development Based on NEP 2020 and LOCF**" held on 23-06-2021 organized by School of Basic Sciences, Central University of Haryana, Mahendergarh, Haryana, India.

Computational Experience:

- Expert level of training in softwares: Gaussian 09, ORCA, Jaguar, ADF, Molecular Docking etc
- Visualization: Chemcraft, Maestro, Molekel, Molden, Gaussview, Avogadro, Chimera etc
- Operating Systems: LINUX, WINDOWS

Teaching Interests at Central University of Haryana:

- Computational Chemistry

- Spectroscopy & Photoinorganic Chemistry
- Analytical Chemistry
- Organometallic Chemistry
- Coordination Chemistry
- Inorganic Chemistry Practical
- Chemistry of Materials
- Spectroscopic Techniques for Chemists
- Research Methodology