

Dr. AZAJ ANSARI

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Educational Qualifications:

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

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, 17th-18th 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, 6th-9th 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.
- 2nd MCBR Winter School 2015 grant awarded by **University of Heidelberg**, Germany, 2015.

Additional Charge at Central University of Haryana:

- Liaison officer
- Assistant proctor
- Faculty coordinature in equal opportunity cell
- Faculty representative in anti-ragging
- Standing committee member for admissions
- Committee member for making a roaster for teaching and non-teaching posts
- Departmental research committee member
- Student advisor

Visiting Theoretical Scientist:

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

List of Project:

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

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 Assistant

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

List of Ph.D. Students (Ongoing):

1. **Ms. Monika:** Project titled "A Density Functional Theory Approach Towards Electronic Structures of High-Valent Metal Species and Metal Mediated Catalytic Transformation Reactions".
2. **Ms. Oval Yadav:** Project titled "A Computational Study on High-valent Metal Mediated Catalytic Transformation Reactions".

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

1. Under-graduate project: dissertation title "*A Brief Introduction to Computational Chemistry*" by Mr. Amit Kumar.
2. Under-graduate project: dissertation title "*A Computational Approach on High-valent Non-heme Iron-oxo Complexes*" by Ms. Manisha Kumari.
3. Under-graduate project: dissertation title "*Computational studies of characterization of iron-oxo compound*" by Mr. Navneet Sharma.
4. Under-graduate project: 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. Under-graduate project: dissertation title "*Spectroscopic Characterization of High Valent Iron(III/IV)-oxo Complexes*" by Ms. Sunita Kumari.

6. Under-graduate project: 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. Under-graduate project: dissertation title “*Electronic Structure of Manganese (II) complex $[(Mn(N_3Py_2)]^{n+}$* ” by Ms. Trishtha.
9. Under-graduate project: dissertation title “*A Computational Approach Towards Oxygenation of Cyclohexene by an Iron(V)-Oxo Complex*” by Ms. Hemlata.
10. Under-graduate project: dissertation title “*Reactivity of an Iron(IV)-Oxo Complex with Protons and Oxidants: A DFT Exploration*” by Mr. Rahul Yadav.
11. Under-graduate project: dissertation title “*Electronic Structure and Reactivity of Co^{II} -OH Complexes*” by Mr. Bhanu Pratap.

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 Symposium 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***”.
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*”.

Extension Lecture:

- “*Role of High-valent Metal-oxo Species in Catalytic Reactions?*” Government College, Narnaul, Haryana, 4th February 2017.

National Conference as an Organizer:

- *Recent Trends in Eco-Friendly Chemistry (RTEC 2016)*, September 29, 2016 at Central University of Haryana, Mahendergarh, Haryana.

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. (**Impact Factor = 13.858**)
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. (**Impact Factor = 4.029**)
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. (**Impact Factor = 4.123**)
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. (**Impact Factor =**)
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. (**Impact Factor = 11.994**)
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. (**Impact Factor = 1.235**)
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. (**Impact Factor = 4.029**)

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. (**Impact Factor = 4.857**)
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 and Gopalan Rajaraman *Chem. Eur. J.* **2017**, 23, 10110. (‡equal contribution) (**Impact Factor = 5.317**)
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**[‡] and Gopalan Rajaraman *Chem. Eur. J.* **2018**, 24, 6818. (‡ equal contribution). (**Impact Factor = 5.317**)
11. "Axial vs. Equatorial Ligand Rivalry in Controlling the Reactivity of Iron(IV)-Oxo Species: Single-State vs. Two-State Reactivity" Ravi Kumari[‡], **Azaj Ansari**[‡] and Gopalan Rajaraman *Chem. Eur. J.* **2018** (‡ both authors contributed equally to this article). (**Impact Factor = 5.317**) (List of UGC approved Journals (S.No. 5509) and refereed journal.)
12. "Role of High-valent Metal-oxo vs. superoxo Towards C-H Bond Reactivity: A Computational Investigation" **Azaj Ansari** (*Manuscript under preparation*).
13. "Electronic Structures, Spectroscopic and Reactivity of High-valent Fe/Mn-oxo/hydroxo Complexes: A Computational Exploration" **Azaj Ansari** (*Manuscript under preparation*).
14. "A Comparable Computational Understanding on the Structure, Spin-state Energetics and Spectroscopic Parameters of Heme and Non-heme Complexes towards Aliphatic Hydrocarbons" **Azaj Ansari** (*Manuscript under preparation*).

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 Theoretical 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 February 2014.
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.
15. “*Conference on Modern Trends in Molecular Magnets (MTMM)*” 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.

Computational Experience:

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

As a Reviewer:

- Journal of Central University of Haryana – 2
- Chiang Mai Journal of Science - 1

Teaching Assistantship at IIT Bombay:

CH-117L - Chemistry lab for undergraduate students (January 2012 – December 2012).

Teaching Interests at Central University of Haryana:

- SCSC 401A CHEM 3003 Spectroscopy & Photoinorganic Chemistry
- SCS CH 1 1 01 DCEC 4004 Analytical Chemistry
- SCS CH 1302 DCEC 4004 Advanced Computational Chemistry

- SCS CH 1 1 01 C 4004 Inorganic Chemistry-I
- SCS CH 1 2 05 C 4004 Inorganic Chemistry-II (Organometallic Chemistry)
- SCS CH 1201 C 4004 Inorganic Chemistry-II (Coordination Chemistry)
- SCS CH 1 1 04 C 0044 Chemistry Laboratory-I
- SCS CH 1110 GE 4004 Chemistry of Materials
- SCS CH 3107 E 6006 Spectroscopic Techniques for Chemists