

CURRICULUM VITAE

RAHUL KUMAR, PhD

Former Postdoctoral Research Associate
Pacific Northwest National Laboratory
Mob. No. +91-8448774033
e-mail: rkiisc@gmail.com

Address: B-19 (2nd Floor)
Block-B, RWA, Sector-122
Gautam Budh Nagar, Noida-201301
Uttar Pradesh, India

RESEARCH INTERESTS

- **Catalysis and Material Science for Renewable Energy and Sustainability:**
 - **Thermal/Electro/Photo Catalysis and Surface Chemistry for**
 - Biomass upgradation to fuels and chemicals using biorefinery
 - Green House Gases($\text{CH}_4 + \text{CO}_2$) conversion to C1-C2 feed stocks
 - Plastic upcycling into value added chemicals and fuels
 - **Materials for H_2 storage and Electronics**
 - **Computational Chemistry**
 - DFT calculation for molecular/electronic properties and mechanistic insights

PROFESSIONAL EXPERIENCE

- **July 2018–January 2021, Postdoctoral Research Associate**
 - Heterogenous catalysis and Surface Chemistry, Green and Sustainable Chemistry
 - Pacific Northwest National Laboratory (**PNNL**), Richland, WA, USA
 - **Mentors:** Dr. Tom Autrey and Dr. Abhi Karkamkar
 - **Project Title:** (i) Using calorimetry to measure energy landscape of aqueous phenol reduction catalyzed by Ru/C (ii) Calorimetry to measure heat of adsorption of hydrogen on Pt-black, Pt/C, and Pt/SiO₂ under water and other solvents and with pH
- **March 2017–March 2018, National Postdoctoral Fellow(N-PDF) and Co-PI**
 - Inorganics Organometallics: Main Group chemistry
 - **TIFR**, Hyderabad (**TCIS**), India
 - **PI and Mentor:** Dr. Anukul Jana
 - **Project Title:** (i) Rational Design for the synthesis of P-Si triple bond and (ii) Stabilization of Mg(0)-NHCs complexes
- **April 2016–February 2017, Postdoctoral Research Associate**
 - Computational Chemistry: DFT Calculation
 - Dept. of Inorganic and Physical Chemistry (**IPC**), Indian Institute of Science (**IISc.**), Bangalore, India
 - **Mentor:** Prof. E. D. Jemmis

- **Project title:** (i) Computational studies on the investigation of CH₄ activation pathways through O₂ activation using metal-peroxo complexes and (ii) Multiple bonding between heavier main group elements.

EDUCATION

- **January 2011–July 2016, Ph.D.,**
 - Inorganic and Organometallic chemistry
 - Indian Institute of Science (**IISc.**), Dept. of IPC, Bangalore, India
 - **Ph.D. Thesis title:** Mechanistic insights into the small molecule [amine-boranes (R₂HN·BH₃), hydrogen (H₂), methane (CH₄), formic acid (HCOOH) and carbon dioxide (CO₂)] activation using electrophilic Ru(II)-complexes
 - **Research Advisor:** Prof. B. R. Jagirdar,
- **August 2007–December 2010, M.S. Chemistry**
Indian Institute of Science (**IISc.**), Dept. of IPC, Bangalore, India
 - **Project title:** B-H bond activation of amine-boranes using [Ru(Cl)(dppe)₂][OTf] complex
 - **Research Advisor:** Prof. B. R. Jagirdar
- **August 2004–July 2007, B.Sc.(Honors) in Chemistry, [University rank: 2nd]**
 - Banaras Hindu University (**BHU**), Varanasi, India

AWARDS, HONORS AND ACHIEVEMENTS

- **Outstanding Performance Award** for scientific excellence in catalysis science
November 2020, PNNL
- **American Chemical Society (ACS)** award of "**Certificate of Recognition**" for the valued contribution to ACS as a **reviewer**, March 2019, from Dr. Sarah Tegen, Vice President, Global Editorial & Author Services at ACS
- **National Postdoctoral Fellowship (N-PDF)**, January 2017 SERB (Science and Engineering research board of India)
- **Best poster award** for the research paper "Implication of a σ-methane complex en route to elimination of methane from a ruthenium complex: An experimental and theoretical investigation" December 2014, **Theoretical Chemistry Symposium**, Pune, India
- **SERB Travel Grant** awarded to attend prestigious **Gordon Research Conference, Organometallic chemistry 2015**, Salve Regina University, Rhode Island, USA

- **CSIR NET (Chemical Sciences)** qualified, **December 2009**
- **IIT JAM MSc (Chemistry) 2007** written exam qualified and got the offer for admission from **IIT Delhi**
- **Qualified IISc, Bangalore Int.Ph.D. program (Chemical Sciences) 2007** written test and two rounds of interviews qualified
- **JNU, New Delhi MSc (Biotech) 2007** written exam qualified
- **BHU, UET(B.Sc.) 2004 and PET(MSc) (Chemistry) 2007** entrance exam qualified

PUBLICATIONS

1. A detailed energy landscape describing the catalytic hydrogenation of phenol to cyclohexanol using Ru/C in the aqueous media, **Rahul Kumar**, Yang Yu, Teng He, Udishnu Sanyal, Katherine Koh, Abhi Karkamkar, Oliver Y. Gutiérrez, Donald M. Camaioni, Tom Autrey Manuscript Under Review to *Journal of Catalysis*.
2. Mechanistic Insights into Formic Acid Dehydrogenation and Carbon dioxide Amidation Using Electrophilic Ru(II)-Complexes **Rahul Kumar** and Balaji R. Jagirdar, manuscript Under revision (after reviewer's suggestion) to *Journal of Organometallic Chemistry*.
3. Solid-state hydrogen rich boron–nitrogen compounds for energy storage, **Rahul Kumar**, Abhi Karkamkar, Mark Bowden, Tom Autrey, *Chem. Soc. Rev.* **2019**, 48, 5350–5380
4. Implication of a σ -methane complex en route to elimination of methane from a ruthenium complex: An experimental and theoretical investigation, **Rahul Kumar**, R. Shyama, Eluvathingal D. Jemmis, and Balaji R. Jagirdar *Organometallics*, **2015**, 34, 1245–1254
5. B–H Bond activation using an electrophilic metal complex: Insights into the reaction pathway, **Rahul Kumar** and Balaji R. Jagirdar, *Inorg. Chem.*, **2013**, 52, 28–36.

TECHNICAL EXPERTISE

- Basics of Electrochemistry, Surface Chemistry, Catalysis (Heterogeneous and Homogeneous) Calorimetry and high-pressure reactions using Parr reactor and autoclave

- Probing reaction mechanism using chemical kinetics and thermodynamics, spectroscopy and DFT calculations
- Manipulation of highly sensitive compounds using Schlenk Line and Glove Box Techniques
- Synthesis of Organometallic complexes & Nanoparticles (catalysts), inorganic and organic compounds
- NMR Spectroscopy: 2D NMR (COSY, NOESY, HETCOR), Variable temperature (VT) and high-pressure NMR spectroscopic techniques
- Analysis and characterization of chemical compounds using NMR, IR, UV-Vis spectroscopy and X-ray crystallography
- Programming language: Fortran (90, 95)
- Operating systems: Linux, MacBookPro, Windows XP and 10 pro.
- Software: Microsoft package: ChemDraw & ProFit, Topspin (NMR), Gaussian 09, CCDC, Mercury, SciFinder, Web of Sciences etc.

CONFERENCES/SYMPOSIA/SEMINARS

- Oral Presentation “Calorimetry to explore the kinetics and thermodynamics of phenol hydrogenation by heterogeneous metal catalysts”, ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY (ACS) SYMPOSIUM, **August 25-29, 2019**, San Diego, California
- Poster presentation “Calorimetry to Explore the Kinetics and Thermodynamics of Phenol Hydrogenation By Heterogeneous Metal Catalysts”, 2019 NORTH AMERICAN CATALYSIS SOCIETY (NAM26) MEETING, **June 23 - 28, 2019**, Chicago, Illinois
- SERB N-PDF invited seminar at TIFR, Hyderabad, **March, 2017** for the postdoctoral research project on “Rational design for the synthesis of P-Si triple bond and (ii) Stabilization of Mg(0)-NHCs complexes”
- Participated in **Recent Advances in Theoretical Chemistry, Dept. of IPC, at IISc., Bangalore, Jul 8-9, 2016**
- Participated in **ACS on campus-IISc mini-symposium at IISc., Bangalore, Jan 27, 2016**
- Presented a poster entitled “Approaches toward σ -borane and σ -methane complexes of ruthenium” in **Gordon Research Conference/Seminar (GRC and GRS), Organometallic Chemistry, 11th-17th July 2015** held at **Salve Regina University, Newport, Rhode Island, USA**

- Oral Presentation on “An Approach towards C-H Bond activation of methane using Ru(II) complex” in **In-House Symposium** in 27th September **2014** at **Department of Inorganic and Physical Chemistry (IPC), IISc., Bangalore.**
- Presented a poster in “Mechanistic insights into B-H Bond activation of amine-boranes using electrophilic Ru(II)-complex” **3rd Asian Coordination Chemistry Conference** in October **2012**, organized by **Indian Institute of Technology (IIT), Delhi and Kanpur, India.**
- Oral Presentation on “Ammonia-Borane as hydrogen storage material: its dehydrogenation using organometallic complexes” in **Student Seminar Series** in September **2011, IPC, IISc., Bangalore, India**
- Oral Presentation on “Controlling motion at molecular level: the molecular machines” in **Student Seminar Series** in August **2010, IPC, IISc., Bangalore, India**
- The **International Hydrogen Storage Conference**, 3rd -6th January **2009**, Division of Chemical Sciences, Indian Institute of Science (**IISc.**), Bangalore, India. (Convener Prof. B. R. Jagirdar).
- The **IISc. Centenary Conference**, 13th-16th December **2008**, Indian Institute of Science (**IISc.**), Bangalore, India held for celebrating **100 years of IISc.**