

RAHUL KUMAR, PhD

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HIGHLIGHTS: I am a **Chemist** and **R&D project manager** by research experience. Have total **10.5 years** of research time in the **R&D sectors** of premier research institutions in India and USA (Vide infra). In the time frame of about a decade devoted to research, I have worked on **fundamentals and applied CATALYSIS** research projects focused on

1. GREEN & SUSTAINABLE ENERGY
2. BIOMASS VALORIZATION

During this time span, I have acquired knowledge & expertise in the following areas:

- **Design, Development and Management of Research Projects** and R&D Labs focused on
 - Transformation of **Green House Gases (CH_4 & CO_2)** into **C1-C2** feed stocks
 - **Biomass upgradation & Waste Plastic upcycling**
 - **H₂ storage & production**
- **Safety protocols for**
 - **R&D labs working on High Energy Fuels**, pressurized gases and chemicals (such as **H₂, CH₄, CO₂, CO, CH₃OH** etc.)
- **Good writing and communication skills** reflected in the presentations (conferences, symposia and seminars); published & drafted research papers for H₂ storage & release for fuel cell applications, CH₄ & CO₂ transformation to C1-C2 feedstock and Biomass valorization.

Currently, I am actively looking for job opportunities such as Assistant Professor, R&D Scientist, Research Associate and Project Manager

RESEARCH INTERESTS

- **Catalysis for Renewable Energy, Climate Change & Sustainability:**
 - Biomass upgradation to fuels and chemicals using biorefinery
 - Green House Gases (CH_4 + CO_2) conversion to C1-C2 feed stocks
 - Plastic upcycling into value added chemicals
- **Materials for reversible H₂ storage**

PROFESSIONAL EXPERIENCE

- **July 2018–January 2021, Postdoctoral Research Associate**
 - **Specialization:** Heterogenous catalysis and Surface Chemistry, Biomass valorization Green and Sustainable Chemistry

- **Institute:** 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**
 - **Specialization:** Inorganics Organometallics: Main Group chemistry
 - **Institute:** Tata Institute of Fundamental Research (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**
 - **Specialization:** Computational Chemistry & DFT Calculation
 - **Institute:** 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. in Chemistry**
 - **Specialization:** Inorganic and Organometallic chemistry (Green & Sustainable Energy, Catalysis)
 - **Institute:** Dept. of Inorganic and Physical Chemistry (IPC), Indian Institute of Science (IISc.), 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. in Chemistry**
Institute: Dept. of IPC, Indian Institute of Science (IISc.), Bangalore, India
 - **Project title:** B-H bond activation of amine-boranes using $[\text{Ru}(\text{Cl})(\text{dppe})_2][\text{OTf}]$ complex
 - **Research Advisor:** Prof. B. R. Jagirdar
- **August 2004-July 2007, B.Sc.(Honors) in Chemistry**
 - **Institute:** 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*, 2021.

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*, 2021.
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

- Surface Chemistry, Catalysis (Heterogeneous and Homogeneous), Basics of Electrochemistry, Calorimetry and high-pressure reactions using Parr reactors and autoclaves
- 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.**