

PERSONAL DETAILS

Present Address: 2560 Carpenter Rd,
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Date of birth: September 12, 1987

Nationality: Indian

Marital status: Married

Permanent Address: Kalyan Nagar East (Sabuj Sangha Club)
P.O: Kalyan Nagar, P.S: Khardah
North-24-Pargona, West Bengal
India, PIN:700112

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RESEARCH INTEREST

- Developing strategies for **chemical hydrogen storage**
- **N₂** activation through **surface/heterogeneous catalysis**
- Mechanistic investigation of **homogeneous catalysis related to main group chemistry**
- Mechanistic investigation of **O₂** activation by **non-heme Iron(II) dioxygenase enzyme**
- Methanol production through **CO₂ hydrogenation**
- Developing **Lewis and Bronsted Acid Catalyzed Carbonyl-Olefin Metathesis**
- Developing catalytic **Stereoselective, Iterative Glycosylation**

SKILLS

- **Softwares:** Gaussian, Orca, Qchem, Mopac, Fdynamo, Gromacs, NCI plot, NBO, Adobe Photoshop etc.
- **Programming Languages:** Fortran 90, GNU plot, Origin, L^AT_EX
- **Operating Systems:** Different Linux distributions (Ubuntu, CentOS), Windows (XP, 7)
- **Communicating medium:** English, Bengali (native), Hindi (Native).

EMPLOYMENT

- **Junior Research Fellow**

Indian Association for the Cultivation of Science (**IACS**), Kolkata, India, *June.2013-since June.2011*

- **Senior Research Fellow**

Indian Association for the Cultivation of Science (**IACS**), Kolkata, India, *August.2017-since June.2013*

- **Postdoctoral Fellow**

University of Michigan (**UMICH**), Ann Arbor, Michigan, USA,
tober.2017

September.2021-since Oc-

EDUCATION

- **Doctor of Philosophy in Chemistry**

Calcutta University, Kolkata, West Bengal, India

August.2017-since June.2011

- **Thesis Title:** Theoretical Exploration Of The Chemistry of Isoelectronic B-N Analogs of Alkane and Alkene
- **Adviser:** Dr. Ankan Paul, Asso. Prof., Indian Association for the Cultivation of Science
- **Area of Study:** Mechanistic (Computational) investigation on the oligo-polymeization of aminoborane
- **Key Courses:** Quantum Mechanics, Electronic Structure Theory, Condensed Matter Physics

- **Master of Science in Chemistry**

Calcutta University, Kolkata, West Bengal, India

Nov.2010-since Aug.2008

- Specialization: **Physical Chemistry**
- Class/Division: 1st class

- **Bachelor of Science in Chemistry**

Calcutta University, Scottish Church College, Kolkata, India

Jun.2008-since Aug.2005

- Major: **Chemistry**; Minor: Mathematics, Physics ; Compulsory: Environmental Science
- Class/Division: 1st class

ACADEMIC HONORS AND AWARD

- Qualified, Senior Research Fellowship by Council of Scientific and Industrial Research, New Delhi, India (2015).
- Qualified, Junior Research Fellowship by Council of Scientific and Industrial Research, New Delhi, India (2010).
- Qualified, Graduate Aptitude Test in Engineering, 2010.

PUBLICATIONS

- “Brønsted-Acid-Catalyzed Intramolecular Carbonyl–Olefin Reactions: Interrupted Metathesis vs Carbonyl-Ene Reaction” **T. Malakar**, P. M. Zimmerman *J. Org. Chem.*, **2021**, *86*, 3008-3016.
- “Combined Theoretical and Experimental Investigation of Lewis Acid-Carbonyl Interactions for Metathesis” **T. Malakar**, C. S. Hanson, J. J. Devery III, P. M. Zimmerman *ACS Catal.*, **2021**, *11*, 4381-4394.

- “Fluoride Migration Catalysis Enables Simple, Stereoselective, and Iterative Glycosylation” G. C. Sati, J. L. Martin, Y. Xu, **T. Malakar**, P. M. Zimmerman, J. Montgomery, *J. Am. Chem. Soc.*, **2020**, *142*, 7235-7242.
- “Unraveling the Crucial Role of Single Active Water Molecule in the Oxidative Cleavage of Aliphatic C–C Bond of 2,4-Dihydroxyacetophenone Catalyzed by 2,4-Dihydroxyacetophenone Dioxygenase Enzyme: A Quantum Mechanics/Molecular Mechanics Investigation” R. Manna, **T. Malakar**, B. Jana, A. Paul, *ACS Catal.*, **2018**, *8*, 10043-10050.
- “Combining protons and hydrides by homogeneous catalysis for releasing desirable extent of hydrogen from Ammonia- Borane: Present Status and Challenges” S. Bhunya, **T. Malakar**, G. Ganguly, A. Paul, *ACS Catal.*, **2016**, *6*, 7907-7934.
- “The Mechanism of Acceptorless Amine Double Dehydrogenation by N,N,N-Amide Ruthenium(II) Hydrides: A Combined Experimental and Computational Study” L. V. A. Hale, **T. Malakar**, K-N. Tseng, P. M. Zimmerman, A. Paul, N. K. Szymczack, *ACS Catal.*, **2016**, *6*, 4799-4813.
- “In Pursuit of Sustainable Hydrogen Storage with Boron-Nitride Fullerene as the Storage Medium” G. Ganguly, **T. Malakar**, A. Paul, *ChemSusChem*, **2016**, *9*, 1386-1391.
- “Theoretical Investigation on the Chemistry of Entrapment of the Elusive Aminoborane $H_2N=BH_2$ Molecule” **T. Malakar**, S. Bhunya, A. Paul, *Chem. Eur. J.* **2015**, *21*, 6340-6345. [Hot Paper \(Frontispiece\)](#)
- “Theoretical Studies on the Mechanism of Homogeneous Catalytic Olefin Hydrogenation and Amine–Borane Dehydrogenation by a Versatile Boryl-Ligand-Based Cobalt Catalyst ” G. Ganguly, **T. Malakar**, A. Paul, *ACS Catal.*, **2015**, *5*, 2754-2769.
- “Unfolding the crucial role of a nucleophile in Ziegler–Natta type Ir catalyzed polyaminoborane formation” S. Bhunya, **T. Malakar**, A. Paul, *Chem. Commun.*, **2014**, *50*, 5919-5922.
- “Dramatic reduction in the activation barrier for dinitrogen splitting using amine–borane as a hydrogen carrier: insights from the DFT study” **T. Malakar**, A. Paul, *Chem. Commun* **2014**, *50*, 2187-2189.
- “The Role of Solvent and of Species Generated in Situ on the Kinetic Acceleration of Aminoborane Oligomerization” **T. Malakar**, L. Roy, A. Paul, *Chem. Eur. J.* **2013**, *19*, 5812-5817.
- “Copper(II) Complexes of 3,4,5-Trisubstituted Pyrazolates: InSitu Formation of Pyrazole Rings from Different Carbon Centers” O. Das, **T. Malakar**, A. Mandal, A. Paul, T. K. Paine *Chem. Asian. J.* **2013**, *8*, 623-629.

PUBLICATIONS - IN PROCESS

- “Combined Theoretical and Experimental Investigation of By-Product Inhibition in COM Reactions ” **T. Malakar**, J. J. Devery III, P. M. Zimmerman *Manuscript in preparation*

PROFESSIONAL DEVELOPMENT

- **Conferences & Posters:**
 - Recent Advances in Many Electron Theories (RAMET II), (December 1 - 4, 2011), Puri, India.
 - Current Trends in Theoretical Chemistry (CTTC 2013), (September 26 - 28, 2013), BARC, Mumbai, India. Presented a poster titled “Overcoming the Haber-Bosch Hurdle ”

- Electronic Structure and Dynamics of Molecules and Cluster (ESDMC 2013), (February 17 - 20, 2013), IACS, Kolkata, India.
- From the Chemical Bond to the Chemical Plant, Computational and materials challenges in gas conversion technologies (August 25 - 28, 2014), JNCASR, Bangalore, India. Presented a poster titled **“Designing a Main-Group Molecular Vehicle for Hydrogen Delivery”**. ”
- Workshop on Electronic Structure, Atomistic and Statistical Modeling in Chemistry, Materials and Life Sciences 2014, (October 20 - 22, 2014), IACS, Kolkata, India.
- Theoretical Chemistry Symposium (TCS 2014), (December 18 - 21, 2014), NCL, Pune, India. Presented a poster titled **“Theoretical Studies on the Mechanism of Homogeneous Catalytic Olefin Hydrogenation and Amine-Borane Dehydrogenation by a Versatile Boryl-Ligand-Based Cobalt Catalyst ”**
- Recent Advances in Many-Electron Theory (RAMET)-2017 , (February 9 - 12, 2017),Goa, India. Presented a poster titled **“From Enzymatic to Bio-mimetic Model : A QM-MM Investigation on the Mechanism of 2,4- Dihydroxyacetophenone Dioxygenase (DAD) ”**
- **Oral Presentations:**
 - **“Theoretical Exploration Of The Chemistry of Isoelectronic B-N Analogs of Alkane and Alkene”**, Open Thesis Colloquium, August 23, 2016, IACS, Kolkata, India
 - **“Achieving Catalytic Carbonyl-Olefin Metathesis: Switching the Mechanism and Outcome with Change of Acid”**, 40th Annual MC-NACS Spring Symposium, May 07, 2019, Henry Ford Museum in Dearborn, MI, USA
 - **“Understanding Catalyst Inhibition in Metathesis: High Coordinate Lewis Acid-Carbonyl Complexes ”**, ACS Spring Symposium, May 14, 2021

REFERENCES

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