

Curriculum Vitae of Dibyendu Mallick

Dr. Dibyendu Mallick

Assistant Professor, Department of Chemistry, Presidency University, Kolkata

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Homepage : NA

Research Interests/Specialization:

Computational Bio-inorganic Chemistry

- Reactivity of Metalloenzymes and Bio-mimetic Catalysts
- C-H, N-H and O-H Bond Activation by Organometallic Catalyst.
- Electronic Structure and Bonding of Exotic Molecules

Education and Training:

- **2014-2017:** Postdoctoral Research Fellow; The Hebrew University of Jerusalem Israel.
- **2013-2014:** Postdoctoral Research Associate; Indian Institute of Science (IISc), Bangalore.
- **2008-2013:** Ph.D.; Indian Institute of Science (IISc), Bangalore.
- **2005-2008:** M.S. (Integrated Ph.D.) Chemical Sciences; Indian Institute of Science, Bangalore.
- **2002-2005:** B.Sc. Chemistry (Hons.); The University of Burdwan, West Bengal.

Professional Affiliations:

- **Assistant Professor (Nov 2018 – Present)**
Department of Chemistry, Presidency University, Kolkata
- **Assistant Professor (August 2017 – Oct 2018)**
School of Chemistry and Biochemistry, Thapar University, Patiala
- **PBC Postdoctoral Research Fellow (May 2014 - July 2017)**
Institute of Chemistry, The Hebrew University of Jerusalem Israel.
Advisor: Prof. Sason Shaik
Area of research: Reactivity of Metalloenzymes and C-H, N-H and O-H Bond Activation by Metal-oxo, -hydroxo and -carbene Complexes
- **Postdoctoral Research Associate (October 2013 - April 2014)**
Department of Inorganic & Physical Chemistry, Indian Institute of Science (IISc), Bangalore.
Advisor: Prof. E. D. Jemmis
Area of research: Electronic Structure and Bonding of Main Group Clusters
- **Doctoral (Ph.D.) work (July 2008 - September 2013)**
Department of Inorganic & Physical Chemistry, Indian Institute of Science (IISc), Bangalore.
Advisor: Prof. E. D. Jemmis

Title of thesis: Exploring Structure and Reactions: Computational Studies on Three-Membered Rings, Metal-Boron Multiple Bonds and Biradical Reactions.

Area of research: Electronic Structure and Bonding of Three-membered Ring Systems, Organic Reaction Mechanisms Involving Biradicals.

Teaching Activities:

M.Sc. (Chemistry), Presidency University:

- CHEM1001C: Quantum Chemistry-II
- CHEM1002C: Quantum Chemistry-III
- CHEM0803: Atomic Structure (Hydrogen Atom Part)
- CHEM0892: Computer Applications

B. Sc. Courses

B. Sc. (Chemistry), Presidency University:

- CHEM0401: Quantum Chemistry-I
- CHEM02GE2: Chemical Energetics
- CHEM0691: Advanced Physical Practical

List of Publications (SCI Journals):

1. "Structure and Bonding in Cyclic Isomers of $B_2AlH_n m$ ($n = 3-6$, $m = -2$ to $+1$): A Comparative Study with $B_3H_n m$, $BA_2H_n m$ and $Al_3H_n m$," **D. Mallick**, P. Parameswaran, and E. D. Jemmis, **J. Phys. Chem. A**, **2008**, *112*, 13080-13087. **(Impact Factor: 2.847)**
2. "Which one is preferred: Myers-Saito cyclization of ene-yne-allene or Garratt-Braverman cyclization of conjugated bisallenic sulfone? A theoretical and experimental study," A. Basak, S. Das, **D. Mallick**, E. D. Jemmis, **J. Am. Chem. Soc.**, **2009**, *131*, 15695-15704. **(Impact Factor: 13.858)**
3. "Generation of Cationic Two-Coordinate Group 13 Ligand Systems by Spontaneous Halide Ejection: Remarkably Nucleophilic Resistant (Dimethylamino) borylene Complexes," D. A. Addy, G. A. Pierce, D. Vidovic, **D. Mallick**, Eluvathingal D. Jemmis, J. M. Goicoechea, and Simon Aldridge, **J. Am. Chem. Soc.**, **2010**, *132*, 4586-4588. **(Impact Factor: 13.858)**
4. "Selectivity in Garratt-Braverman Cyclization: An Experimental and Computational Study", M. Maji, **D. Mallick**, S. Mondal, A. Anoop, S. S. Bag, A. Basak and E. D. Jemmis, **Org. Lett.**, **2011**, *13*, 888-891. **(Impact Factor: 6.579)**
5. "Structure-Activity Relationship of Photocytotoxic Iron(III) Complexes of Modified Dipyrrophenazine Ligands", S. Saha, **D. Mallick**, R. Majumdar, M. Roy, R. R. Dighe, E. D. Jemmis, and A. R. Chakravarty, **Inorg. Chem.** **2011**, *50*, 2975-2987. **(Impact Factor: 4.857)**
6. "Remarkable photocytotoxicity in hypoxic HeLa cells by a dipyrrophenazine copper(II) Schiff base thiolate", D. Lahiri, R. Majumdar, **D. Mallick**, T. K. Goswami, R. R. Dighe, A. R. Chakravarty, **J. Inorg. Biochem.** **2011**, *105*, 1086-1094. **(Impact Factor: 3.348)**

7. "Reactivity of Bispropargyl Sulfones under Basic Conditions: Interplay Between Garratt–Braverman and Schmittel/Myers–Saito Cyclization Pathway", R. Mukherjee, S. Mondal, A. Basak, **D. Mallick**, E. D. Jemmis, *Chem. An Asian Journal*, **2012**, 7, 957-965. **(Impact Factor: 4.083)**
8. "(Dimethylamino)borylene and Related Complexes of Electron-Rich Metal Fragments: Generation of Nucleophile-Resistant Cations by Spontaneous Halide Ejection", D. A. Addy, N. Phillips, G. A. Pierce, D. Vidovic, T. Krämer, **D. Mallick**, E. D. Jemmis, G. Reid, and S. Aldridge, *Organometallics*, **2012**, 31, 1092-1102. **(Impact Factor: 3.862)**
9. "Structural Variations in Aromatic 2pi-electron Three Membered Rings of the Main Group Elements", **D. Mallick** and E. D. Jemmis, *J. Chem Sci.* **2015**, 127, 183-196. **(Impact Factor: 1.298)**
10. "Theory Revealing Unusual Non-Rebound Mechanisms Responsible for the Distinct Reactivities of O=MnIV=O and [HO–MnIV–OH]²⁺ in C–H Bond Activation", **D. Mallick** and S. Shaik, *ACS Catal.* **2016**, 6, 2877-2888. **(Impact Factor: 10.614)**
11. "Computation Sheds Insight into Iron Porphyrin Carbenes' Electronic Structure, Formation, and N-H Insertion Reactivity", D. A. Sharon, **D. Mallick**, B. Wang and S. Shaik, *J. Am. Chem. Soc.* **2016**, 138, 9597-9610. **(Impact Factor: 13.858)**
12. "Kinetic Isotope Effect Probes the Reactive-Spin State, as Well as the Geometric Feature and Constitution of the Transition State During H-Abstraction by Heme Compound II Complexes", **D. Mallick** and S. Shaik, *J. Am. Chem. Soc.* **2017**, 139, 11451-11459. **(Impact Factor: 13.858)**
13. "Privileged Role of Thiolate as the Axial Ligand in Hydrogen Atom Transfer Reactions by Oxoiron(IV) Complexes in Shaping the Potential Energy Surface and Inducing Significant H-Atom Tunneling", J. E. M. N. Klein, D. Mandal, W. M. Ching, **D. Mallick**, L. Que, and S. Shaik, *J. Am. Chem. Soc.* **2017**, 139, 18705. **(Impact Factor: 13.858)**
14. "Kinetic Isotope Effect Determination Probes the Spin of the Transition State, Its Stereochemistry, and Its Ligand Sphere in Hydrogen Abstraction Reactions of Oxoiron(IV) Complexes", D. Mandal, **D. Mallick** and S. Shaik, *Acc. Chem. Res.* **2018**, 51, 107. **(Impact Factor: 20.268)**

Book chapters

1. D. Mallick and E. D. Jemmis, "Main Group Metal Clusters", in Comprehensive Inorganic Chemistry II, Eds-J. Reedijk, K. Poppelmeier, Vol. 9, Theory and Methods, Ed., Santiago Alvarez, Page no. 833, Elsevier, **2013**.

Oral and Poster Presentations:

- **2019: Invited speaker;** Internation Conference on Advanced Chemical and Structural Biology (ICACSB-2019), PRIST University, Tamilnadu.

- **2017:** Poster; Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 8), IIT-Bombay
- **2017:** Poster; *Golden Symposium of Lise Meitner Minerva Center for Computational Quantum Chemistry*, The Hebrew university of Jerusalem Israel
- **2016: Invited speaker;** *Computational Modelling of Molecules and Materials (CM3-2016)*, Nainital, India.
- **2015:** Poster; *Lise Meitner Minerva Symposium-2015*, Tel Aviv University.
- **2013:** Poster; *An Indo-German Conference on Modeling Chemical and Biological Reactivity (MCBR-2013)*, NIPER, Mohali, India.
- **2011:** Poster; *An International Conference on Applied Theory On Molecular Systems (ATOMS-2011)*, IICT, Hyderabad, India.
- **2011:** Poster; *The Ninth Triennial Conference of the World Association of Theoretical and Computational Chemists (WATOC 2011)*, Santiago de Compostela, Spain.
- **2010:** Poster; *Discussion Meeting on Theoretical Chemistry (TCS 2010)*, IIT-KANPUR, India.
- **2007:** Poster; *An Indo-German Conference on Modeling Chemical and Biological Reactivity (MCBR-2007)*, IICT, Hyderabad, India.

Awards/Honours/Fellowships:

- **2014: The PBC Fellowship** for **Outstanding Postdoctoral Researcher** in Israel.
- **2014: 1st Prize** of 2013 Eli Lilly **Outstanding Thesis Award**
- **2011:** International travel grant; Department of Science & Technology (DST), New Delhi.
- **2011: Best poster Award** in An International Conference on Applied Theory On Molecular Systems (ATOMS-2011) at IICT, Hyderabad, India.
- **2009:** A. R. Vasudevamurthy-S. Soundararajan prize for **best student seminar**; IPC, IISc, Bangalore.
- **2007: Junior research Fellow** and eligibility for Lectureship awarded by the Council of Scientific and Industrial Research (CSIR), New Delhi.
- **2005: Best outgoing student award** at Sree Gopal Banerjee College, Bagati for securing highest marks in chemistry (Hons.)

Sponsored Research Projects: NA

Other Professional Activities:

- Served as a reviewer for international journals namely, ACS Catalysis, Journal of Physical Chemistry A.