Mukunda Mandal

5735 S Ellis Ave (Gagliardi Group) – Chicago, IL 60637 – United States
mukunda.chem@gmail.com • www.mukundamandal.com • R8yOJWoAAAAJ

Professional Positions

The University of Chicago *Chicago, IL*
Postdoctoral Researcher 2023 – Present
PI: Prof. Laura Gagliardi

Max Planck Institute for Polymer Research (MPI-P) *Mainz, Germany*
Alexander von Humboldt Postdoctoral Fellow 2020 – 2023
PI: Dr. Denis Andrienko

CSIR-National Chemical Laboratory (NCL) *Pune, India*
Research Internship in Chemistry 2014 – 2015
PI: Prof. Debashree Ghosh

Education

University of Minnesota (UMN) *Twin Cities, MN*
Ph.D. in Chemistry • *GPA: 3.94/4.00* 2015 – 2020
Advisor: Prof. Christopher J. Cramer

Indian Institute of Technology Bombay (IITB) *Mumbai, India*
M.Sc. in Chemistry • *GPA: 9.44/10.00* 2012 – 2014
Advisor: Prof. G. Naresh Patwari

Ramakrishna Mission Residential College, Narendrapur (RKMRC) *Kolkata, India*
B.Sc. in Chemistry • *Marks: 87.25%* 2009 – 2012

Fellowships and Awards

- **Kharasch Postdoctoral Travel Award** *UChicago*
  Departmental travel grant to attend ACS Spring 2024 2023
- **Alexander von Humboldt Fellowship** *MPI-P, Mainz*
  Postdoctoral fellowship for conducting research in Germany 2021 – 2023
- **Doctoral Dissertation Fellowship** *University of Minnesota*
  Awarded to the University's most accomplished doctoral candidates 2019 – 2020
- **INSPIRE Scholarship** *DST, India*
  Presented to exceptional Bachelor's/Master's students in India 2010 – 2014
- **Dr. Sailendra Jha Memorial Prize** *RKMRC, Narendrapur*
  For securing second place with first-class honors in B.Sc. 2012
- **Merit-Cum-Means Scholarship** by Govt. of West Bengal, IN 2008 – 2012

Scholastic Achievements

- **Ranked 4^{th}** in Graduate Aptitude Test in Engineering (GATE/Chemistry) 2014
- **Ranked 11^{th}** in CSIR National Eligibility Test (NET/Chemistry) 2013

Publications

First Author Publications

5. **Mandal, M.**;[†,*] Buss, J. A.;[†] Chen, S.-J.; Cramer, C. J.; Stahl, S. S.[*] ([†]Equal contribution, [*]Corresponding author) "Mechanistic Insights into Radical Formation and Functionalization in Copper/*N*-Fluorobenzenesulfonimide Radical-Relay Reactions." *Chem. Sci.* **2023** *(In Press)*
4. **Mandal, M.**; Cramer, C. J.; Truhlar, D. G.; Sauer, J.; Gagliardi, L. "Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metal–Organic Frameworks." *ACS Catal.* **2020**, *10*, 10051.
3. **Mandal, M.**; Elwell, C. E.; Bouchey, C. J.; Zerk, T. J.; Tolman, W. B.; Cramer, C. J. "Mechanisms for Hydrogen-Atom Abstraction by Mononuclear Copper(III) Cores: Hydrogen-Atom Transfer or Concerted Proton-Coupled Electron Transfer?" *J. Am. Chem. Soc.* **2019**, *141*, 17236.
2. **Mandal, M.**; Luke, A. M.; Dereli, B.; Elwell, C. E.; Reineke, T. M.; Tolman, W. B.; Cramer, C. J. "Computational Prediction and Experimental Verification of ϵ-Caprolactone Ring-Opening Polymerization Activity by an Aluminum Complex of an Indolide/Schiff-Base Ligand." *ACS Catal.* **2019**, *9*, 885.
1. **Mandal, M.**; Das, T.; Grewal, B. K.; Ghosh, D. "Feasibility of Ionization-Mediated Pathway for Ultraviolet-Induced Melanin Damage." *J. Phys. Chem. B* **2015**, *119*, 13288.

Contributing Author Publications

18. Liu, J.; De Bastiani, M.; Aydin, E.; Harrison, G. T.; Gao, Y.; Pradhan, R. R.; Eswaran, M. K.; **Mandal, M.**; Yan, W.; Seitkhan, A.; Babics, M.; Subbiah, A. S. *et al.* "Efficient and Stable Perovskite-Silicon Tandem Solar Cells Through Contact Displacement by MgF_x." *Science* **2022**, *377*, 302.
17. Wang, S.; Frisch. S.; Zhang, H.; Yildiz, O.; **Mandal, M.**; Ugur, N.; Jeong, B.; Ramanan, C. *et al.* "Grain Engineering for Improved Charge Carrier Transport in Two-Dimensional Lead-Free Perovskite Field-Effect Transistors." *Mater. Horiz.* **2022**, *9*, 2633.
16. Yuce, H.; **Mandal, M.**; Yalcinkaya, Y.; Andrienko, D.; Demir, M. M. "Improvement of Photophysical Properties of $CsPbBr_3$ and Mn^{2+}:$CsPb(Br,Cl)_3$ Perovskite Nanocrystals by Sr^{2+} Doping for White Light-Emitting Diodes." *J. Phys. Chem. C* **2022**, *126*, 11277.
15. Naujoks, T.; Jayabalan, R.; Kirsch, C.; Zu, F.; **Mandal, M.**; Wahl, J. *et al.* "Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment." *ACS Appl. Mater. Interfaces* **2022**, *14*, 28985.
14. Lee, A. L.; Pandey, A. K.; Chiniforoush, S.; **Mandal, M.**; Li, J. *et al.* "Development of a Highly Responsive Organofluorine Temperature Sensor for ^{19}F Magnetic Resonance Applications." *Anal. Chem.* **2022**, *94*, 3782.
13. Yu, X.; Fu, S.; **Mandal, M.**; Yao, X.; Liu, Z.; Zheng, W.; Samorì, P.; Narita, A.; Müllen, K. *et al.* "Tuning Interfacial Charge Transfer in Atomically Precise Nanographene-Graphene Heterostructures by Engineering van der Waals Interactions." *J. Chem. Phys.* **2022**, *156*, 074702.
12. Lapkin, D.; Kirsch, C.; Hiller, J.; Andrienko, D.; Assalauova, D.; Braun, K. *et al.* "Spatially Resolved Fluorescence of Caesium Lead Halide Perovskite Supercrystals Reveals Quasi-atomic Behavior of Nanocrystals." *Nat. Commun.* **2022**, *13*, 892.

11. Wahl, J.; Engelmayer, M.; **Mandal, M.**; Naujoks, T.; Haizmann, P.; Maier, A.; Peisert, H. *et al.* "Porphyrin Functionalization of $CsPbBrI_2$/ SiO_2 Core-Shell Nanocrystals Enhances the Stability and Efficiency in Electroluminescent Devices." *Adv. Optical Mater.* **2021**, 2101945.
10. Suh, S.-E.; Chen, S.-J.; **Mandal, M.**; Guzei, I.; Cramer, C. J.; Stahl, S. S. "Site-Selective Copper-Catalyzed Azidation of Benzylic C–H Bonds." *J. Am. Chem. Soc.* **2020**, *142*, 11388.
9. Hu, H.; Chen, S.-J.; **Mandal, M.**; Pratik, S. M.; Buss, J. A.; Krska, S. W.; Cramer, C. J.; Stahl, S. S. "Copper-Catalysed Benzylic C–H Coupling with Alcohols via Radical Relay Enabled by Redox Buffering." *Nat. Catal.* **2020**, *3*, 358.
8. Luke, A. M.; Peterson, A.; Chiniforoush, S.; **Mandal, M.**; Popowski, Y.; Sajjad, H. Bouchey, C. J. *et al.* "Mechanism of Initiation Stereocontrol in Polymerization of *rac*-Lactide by Aluminum Complexes Supported by Indolide-Imine Ligands." *Macromolecules* **2020**, *53*, 1809.
7. Elwell, C. E.; **Mandal, M.**; Bouchey, C. J.; Que, L., Jr.; Cramer, C. J.; Tolman, W. B. "Carboxylate Structural Effects on the Properties and Proton-Coupled Electron Transfer Reactivity of $[CuO_2CR]^{2+}$ Cores." *Inorg. Chem.* **2019**, *58*, 15872.
6. Otake, K. I.; Ye, J.; **Mandal, M.**; Islamoglu, T.; Buru, C. T.; Hupp, J. T. *et al.* "Enhanced Activity of Heterogeneous Pd(II) Catalysts on Acid Functionalized Metal-Organic Frameworks." *ACS Catal.* **2019**, *9*, 5383.
5. Saxon, D. J.; Nasiri, M.; **Mandal, M.**; Maduskar, S.; Dauenhauer, P. J. *et al.* "Architectural Control of Isosorbide-Based Polyethers via Ring-Opening Polymerization." *J. Am. Chem. Soc.* **2019**, *141*, 5107.
4. Macaranas, J. A.; Luke, A. M.; **Mandal, M.**; Neisen, B. D.; Marell, D. J. *et al.* "Sterically Induced Ligand Framework Distortion Effects on Catalytic Cyclic Ester Polymerizations." *Inorg. Chem.* **2018**, *57*, 3451.
3. Stasiw, D. E.; Luke, A. M.; Rosen, T.; League, A. B.; **Mandal, M.**; Neisen, B. D.; Cramer, C. J. *et al.* "Mechanism of the Polymerization of *rac*-Lactide by Fast Zinc Alkoxide Catalysts." *Inorg. Chem.* **2017**, *56*, 14366.
2. Fieser, M. E.; Sanford, M. J.; Mitchell, L. A.; Dunbar, C. R.; **Mandal, M.**; Van Zee, N. J.; Urness, D. M. *et al.* "Mechanistic Insights into the Alternating Copolymerization of Epoxides and Cyclic Anhydrides using a (Salph)AlCl and Iminium Salt Catalytic System." *J. Am. Chem. Soc.* **2017**, *139*, 15222.
1. Stasiw, D. E.; **Mandal, M.**; Neisen, B. D.; Mitchell, L. M.; Cramer, C. J.; Tolman, W. B. "Why So Slow? Mechanistic Insights from Studies of a Poor Catalyst for Polymerization of ϵ-Caprolactone." *Inorg. Chem.* **2017**, *56*, 725.

Manuscript in Preparation

Wang, S.; **Mandal, M.**; Zhang, H.; Breiby, D. W.; Yildiz, O.; Floudas, G.; Wang, H. I.; Andrienko, D; Bonn, M.; Blom, P. W. M.; Pisula, W.; Marszalek, T. "Odd-Even Alkyl Chain Effect on Structure and Charge Carrier Transport of Two-Dimensional Sn-Based Perovskite Semiconductors." *In preparation*

Research Experience

Postdoctoral Research at UChicago

- Developing an automated approach for selecting active space to perform MCSCF calculations
- Understanding C–H activation reactivity using multireference-based methods

Postdoctoral Research at MPI-P

- Metal-halide perovskites for solar cells, LEDs, and field-effect transistors

- Nanographene/graphene heterostructures
- TADF emitters for single-layer OLEDs

Doctoral Research at UMN

Thesis: Modeling Homo- and Heterogeneous Catalysis with Applications Ranging from Hydrocarbon Activation to the Synthesis of Sustainable Polymers

Research Interests:

- Polymers from biomass-derived monomers
- Metal-based C–H activation reactions relevant in enzymatic processes
- Catalysis using metal-organic frameworks (MOF) as support material

Research Assistant at CSIR-NCL

Project: Computation of ionization potentials of building blocks of eumelanin

Master's Research at IITB

Project: Unconventional hydrogen bonding in aromatic alkynes using time-of-flight mass spectrometry

Oral Presentations (Selected)

7.	(Upcoming) **Mandal, M.**; Xie, H.; Jangid, B.; Khoshooei, M. A.; Kirlikovali, K.; Farha, O. K.; Gagliardi, L. "Computational Exploration of Hydrogenation Catalysis: Metal-Sulfur Active Sites in Metal-Organic Frameworks."	ACS Meeting Spring 2024 , New Orleans, LA	Mar. 2024 (Upcoming)
6.	(Invited) **Mandal, M.** Scott, T. R.; Gagliardi, L. "Multiconfiguration Pair-Density Functional Theory in Catalysis: Propane Dehydrogenation and MOF-Supported C–H Activation."	XXVI International Workshop on Quantum Systems in Chemistry, Physics, and Biology, Jaipur, India	Oct. 2023
5.	**Mandal, M.** "Modeling Sustainability in Chemistry: From Catalysis to Energy Materials."	Humboldt Salon, *Institute of Molecular Biology*, Mainz, Germany	Jul. 2022
4.	**Mandal, M.**; Cramer, C. J.; Truhlar, D. G.; Sauer, J.; Gagliardi, L. "Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metal–Organic Frameworks."	Inorganometallic Catalyst Design Center, *All-Hands Meeting, UMN*, (Virtual)	Oct. 2020
3.	**Mandal, M.**; Elwell, C. E.; Tolman, W. B.; Cramer, C. J. "Mechanisms for Hydrogen-Atom Abstraction by Reactive Copper(III) Cores: HAT or cPCET?"	Quantum Bio-Inorganic Chemistry Conference, Marseille, France	Jul. 2019
2.	**Mandal, M.**; Elwell, C. E.; Tolman, W. B.; Cramer, C. J. "HAT *vs* cPCET Mechanisms for C–H Bond Activations by LCu(III)–OH, –OOR, and $-O_2CR$ Compounds."	257th ACS National Meeting & Exposition, Orlando, FL	Apr. 2019
1.	**Mandal, M.**; Dunbar, C. R.; Cramer, C. J. "Theory for Mechanistic Analysis and Catalyst Design."	Center for Sustainable Polymers, *Annual Meeting,* Minneapolis, MN	May 2017

Poster Presentations (Selected)

5.	**Mandal, M.**; Wahl, J.; Kirsch, C.; Naujoks, T.; Engelmayer, M.; Lapkin, D.; Vartanyants, I. A.; Liu, J.; Wolf, D. S.; Brütting, W.; Scheele, M.; Andrienko, D. "Modeling Metal–Halide Perovskites for Energy Applications."	SPP-2196 Workshop , *Gustav Stresemann Institute,* Bonn, Germany	Mar. 2023
4.	**Mandal, M.**; Ye, J.; Otake, K. I.; Islamoglu, T.; Buru, C. T.; Hupp, J. T.; Delferro, M.; Farha, O. K.; Truhlar, D. G.; Cramer, C. J. "Computational Characterization of Heterogeneous Pd(II) Catalysts on Acid Functionalized Metal-Organic Frameworks."	Annual PI Meeting, *Energy Frontier Research Center,* Washington, D.C.	Aug. 2019

3. **Mandal, M.**; Luke, A. M.; Macaranas, J. A.; Stasiw, D. E.; Dereli, B.; Reineke, T. M.; Tolman, W. B.; Cramer, C. J. "Mechanistic Analysis and Catalyst Design for Sustainable Polymer Production." — 257th ACS National Meeting & Exposition, Orlando, FL — Apr. 2019
2. **Mandal, M.**; Saxon, D. J.; Fieser, M. E.; Tolman, W. B.; Reineke, T. M.; Cramer, C. J. "*In silico* Catalyst Design for Developing Sustainable Polymers." — CSP Reverse Site Visit, *National Science Foundation,* Alexandria, VA — Mar. 2019
1. **Mandal, M.**; Dereli, B.; Luke, A. M.; Macaranas, J. A.; Stasiw, D. E.; Tolman, W. B.; Cramer, C. J. "Computationally Guided Polymerization Catalyst Design." — Center for Sustainable Polymers, *Annual Meeting,* Minneapolis, MN — Apr. 2018

Professional Activities

Teaching

- Gave a lecture at a graduate-level quantum chemistry course at *UChicago* — 2023
- Undergraduate general chemistry laboratory at *Department of Chemistry, UMN* — 2015 – 2016
- High school general chemistry course at *Bikrampur High School, WB, India* — Summer 2012 & 2013

Grant Writing

- Collaboratively authored two successful grant proposals (DFG & CRG) alongside Dr. Denis Andrienko and a multidisciplinary team during my tenure at MPI-P — 2022
- Secured funding from the Alexander von Humboldt Foundation for an independent postdoctoral research — 2021

Mentorship

- Offered mentorship to Serina Tressler, a graduate student in the Gagliardi group at UChicago, assisting her in conducting independent research — 2023
- Mentored Anika Ahluwalia, a student in the Cramer group at UMN to help conduct independent research — 2017 – 2018

Peer Review

- *Peer-reviewed articles for:* J. Phys. Chem. Lett; J. Org. Chem.; Front. Chem.; R. Soc. Open Sci.

Outreach

- *Volunteer, Minnesota State Fair:* Three consecutive years of involvement with the outreach program of the NSF Center for Sustainable Polymers to educate visitors about bio-based polymers — Summer 2016 – 2018

References

Prof. Christopher J. Cramer
Distinguished McKnight Professor Emeritus
University of Minnesota
E-mail: cramer@umn.edu

Prof. Laura Gagliardi
Richard and Kathy Leventhal Professor
The University of Chicago
E-mail: lgagliardi@uchicago.edu

Prof. Debashree Ghosh
Professor
Indian Association for the Cultivation of Science
E-mail: pcdg@iacs.res.in

Dr. Denis Andrienko
Group Leader, Polymer Theory Group
Max Planck Institute for Polymer Research, Mainz
E-mail: denis.andrienko@mpip-mainz.mpg.de