

Mukunda Mandal

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Professional Positions

The University of Chicago Postdoctoral Researcher	<i>Chicago, IL</i> 2023 – Present
Max Planck Institute for Polymer Research (MPI-P) Alexander von Humboldt Postdoctoral Fellow	<i>Mainz, Germany</i> 2020 – 2023
CSIR-National Chemical Laboratory (NCL) Research Internship in Chemistry	<i>Pune, India</i> 2014 – 2015

Education

University of Minnesota (UMN) Ph.D. in Chemistry GPA: 3.94/4.00	<i>Twin Cities, MN</i> 2015 – 2020
Indian Institute of Technology Bombay (IITB) M.Sc. in Chemistry GPA: 9.44/10.00	<i>Mumbai, India</i> 2012 – 2014
Ramakrishna Mission Residential College, Narendrapur (RKMRC) B.Sc. in Chemistry Marks: 87.25%	<i>Kolkata, India</i> 2009 – 2012

Fellowships and Awards

- **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 students (top 1% in India) completing a Bachelor's and/or Master's degree in natural sciences 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 4th in Graduate Aptitude Test in Engineering (GATE)** 2014
An all-India examination for obtaining Ph.D. Fellowship in Chemistry or for a career in chemical R&D
- **Ranked 11th in CSIR National Eligibility Test (NET)** 2013
A competitive entrance test for prospective Ph.D. scholars in India, held nationwide

First Author Publications

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. [doi](#)
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. [doi](#)
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. [doi](#)
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. [doi](#)

Contributing Author Publications

18. Liu, J. *et al.* "Efficient and Stable Perovskite-Silicon Tandem Solar Cells Through Contact Displacement by MgF_x ." *Science* **2022**, *377*, 302. [doi](#)
17. Wang, S.; Frisch, S.; Zhang, H.; Yildiz, O.; **Mandal, M.**; Ugur, N.; Jeong, B.; Ramanan, C.; Andrienko, D.; Wang, H.; Bonn, M.; Blom, P. W. M.; Kivala, M.; Pisula, W.; Marszalek, T. "Grain Engineering for Improved Charge Carrier Transport in Two-Dimensional Lead-Free Perovskite Field-Effect Transistors." *Mater. Horiz.* **2022**, *9*, 2633. [doi](#)
16. Yuce, H.; **Mandal, M.**; Yalcinkaya, Y.; Andrienko, D.; Demir, M. M. "Improvement of Photophysical Properties of CsPbBr_3 and $\text{Mn}^{2+}:\text{CsPb}(\text{Br},\text{Cl})_3$ Perovskite Nanocrystals by Sr^{2+} Doping for White Light-Emitting Diodes." *J. Phys. Chem. C* **2022**, *126*, 11277. [doi](#)
15. Naujoks, T.; Jayabalan, R.; Kirsch, C.; Zu, F.; **Mandal, M.**; Wahl, J.; Waibel, M.; Andreas, O.; Koch, N. *et al.* "Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment." *ACS Appl. Mater. Interfaces* **2022**, *14*, 28985. [doi](#)
14. Lee, A. L.; Pandey, A. K.; Chiniforush, S.; **Mandal, M.**; Li, J.; Cramer, C. J.; Haynes, C. L.; Pomerantz, W. C. K. "Development of a Highly Responsive Organofluorine Temperature Sensor for ^{19}F Magnetic Resonance Applications." *Anal. Chem.* **2022**, *94*, 3782. [doi](#)
13. Yu, X.; Fu, S.; **Mandal, M.**; Yao, X.; Liu, Z.; Zheng, W.; Samorì, P.; Narita, A.; Müllen, K.; Andrienko, D. *et al.* "Tuning Interfacial Charge Transfer in Atomically Precise Nanographene-Graphene Heterostructures by Engineering van der Waals Interactions." *J. Chem. Phys.* **2022**, *156*, 074702. [doi](#)
12. Lapkin, D. *et al.* "Spatially Resolved Fluorescence of Caesium Lead Halide Perovskite Supercrystals Reveals Quasi-atomic Behavior of Nanocrystals." *Nat. Commun.* **2022**, *13*, 892. [doi](#)
11. Wahl, J.; Engelmayer, M.; **Mandal, M.**; Naujoks, T.; Haizmann, P.; Maier, A.; Peisert, H. *et al.* "Porphyrin Functionalization of $\text{CsPbBr}_2/\text{SiO}_2$ Core-Shell Nanocrystals Enhances the Stability and Efficiency in Electroluminescent Devices." *Adv. Optical Mater.* **2021**, 2101945. [doi](#)
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. [doi](#)
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. [doi](#)
8. Luke, A. M.; Peterson, A.; Chiniforush, S.; **Mandal, M.**; Popowski, Y.; Sajjad, H. *et al.* "Mechanism of Initiation Stereocontrol in Polymerization of *rac*-Lactide by Aluminum Complexes Supported by Indolide-Imine Ligands." *Macromolecules* **2020**, *53*, 1809. [doi](#)

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 [CuO₂CR]²⁺ Cores." *Inorg. Chem.* **2019**, *58*, 15872. [doi](#)
6. Otake, K. I.; Ye, J.; **Mandal, M.**; Islamoglu, T.; Buru, C. T.; Hupp, J. T.; Delferro, M.; Truhlar, D. G.; Cramer, C. J.; Farha, O. K. "Enhanced Activity of Heterogeneous Pd(II) Catalysts on Acid Functionalized Metal-Organic Frameworks." *ACS Catal.* **2019**, *9*, 5383. [doi](#)
5. Saxon, D. J.; Nasiri, M.; **Mandal, M.**; Maduskar, S.; Dauenhauer, P. J.; Cramer, C. J.; LaPointe, A. M.; Reineke, T. M. "Architectural Control of Isosorbide-Based Polyethers via Ring-Opening Polymerization." *J. Am. Chem. Soc.* **2019**, *141*, 5107. [doi](#) 
4. Macaranas, J. A.; Luke, A. M.; **Mandal, M.**; Neisen, B. D.; Marell, D. J.; Cramer, C. J.; Tolman, W. B. "Sterically Induced Ligand Framework Distortion Effects on Catalytic Cyclic Ester Polymerizations." *Inorg. Chem.* **2018**, *57*, 3451. [doi](#)
3. Stasiw, D. E.; Luke, A. M.; Rosen, T.; League, A. B.; **Mandal, M.**; Neisen, B. D.; Cramer, C. J.; Kol, M.; Tolman, W. B. "Mechanism of the Polymerization of *rac*-Lactide by Fast Zinc Alkoxide Catalysts." *Inorg. Chem.* **2017**, *56*, 14366. [doi](#)
2. Fieser, M. E.; Sanford, M. J.; Mitchell, L. A.; Dunbar, C. R.; **Mandal, M.**; Van Zee, N. J.; Urness, D. M.; Cramer, C. J.; Coates, G. W.; Tolman, W. B. "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. [doi](#) 
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. [doi](#)

Submitted Manuscript

1. **Mandal, M.**;*[†] Buss, J. A.;[†] Chen, S.-J.; Cramer, C. J.; Stahl, S. S.* "Mechanistic Insights into Radical Formation and Functionalization in Copper/*N*-Fluorobenzene-sulfonimide Radical-Relay Reactions." *Submitted* (*Corresponding author, [†]Equal contribution)

Research Experience

Postdoctoral Research at UChicago.....

PI: Prof. Laura Gagliardi

Research Interests:

- Understanding C–H activation reactivity using multireference-based methods
- Developing an automated approach for selecting active space to perform MCSCF calculations
- Exploring the complex electronic structure of [Fe₄S₄] clusters relevant in biological systems

Postdoctoral Research at MPI-P.....

Group Leader: Dr. Denis Andrienko

Research Interests:

- Metal-halide perovskites for solar cells, LEDs, and field-effect transistors
- Nanographene/graphene heterostructures
- TADF emitters for single-layer OLEDs

Doctoral Research at UMN.....

Advisor: Prof. Christopher J. Cramer

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.....

Advisor: Prof. Debashree Ghosh

Project: Computation of ionization potentials of building blocks of eumelanin

Master's Research at IITB.....

Advisor: Prof. G. Naresh Patwari

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

Oral Presentations (Selected)

5. **Mandal, M.** "Modeling sustainability in chemistry: From catalysis to energy materials."
Humboldt Salon (Rhein-Main region), *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, UMN, *All-Hands Meeting (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 BioInorganic 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 –O₂CR compounds."
ACS National Meeting, *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 Meeting, *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."
Energy Frontier Research Center, PI Meeting, *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."
ACS National Meeting, *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 to 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."
CSP 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 AvH Foundation for an independent postdoctoral research proposal on halide perovskite nanocrystals for LED applications 2021

Mentorship

2017 – 2018

Mentored a high school student in the Cramer group at UMN to help conduct independent research

Peer Review

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

Outreach

Summer 2016 – 2018

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

References

Prof. Christopher J. Cramer

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University of Minnesota
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Prof. Laura Gagliardi

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

Dr. Denis Andrienko

Group Leader, Polymer Theory Group
Max Planck Institute for Polymer Research, Mainz
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