

Mukunda Mandal

EDUCATION

- 2015 – 2020 **University of Minnesota (UMN), Twin Cities, MN, USA**
(Aug) Ph.D. (Chemistry) GPA – 3.94/4.00
- 2012–2014 **Indian Institute of Technology Bombay (IITB), Mumbai, India**
Master of Science (Chemistry), GPA – 9.44/10.00
- 2009–2012 **R. K. M. R. College, Narendrapur, University of Calcutta, India**
Bachelor of Science (Chemistry), Marks – 87.25 % (Honours/Major)

PROFESSIONAL EXPERIENCE

- 2020 (Sep)– **Max Planck Institute for Polymer Research (MPI-P) Mainz, Germany**
Present Postdoctoral researcher with Dr. Denis Andrienko and Prof. Kurt Kremer

RESEARCH EXPERIENCE

- 2020 (Sep)– **Postdoctoral research associate**, Polymer Theory Department, MPI-P Mainz, Germany
Present Advisors: Dr. Denis Andrienko and Prof. Kurt Kremer
Modeling organic/inorganic hybrid perovskite nanocrystals for electroluminescence applications
- 2015–2020 **Doctoral Research Assistant**, Department of Chemistry, UMN
(Aug) Advisor: Prof. Christopher J. Cramer
Computational modeling of catalytic processes involved in:
◦ Sustainable polymer production
◦ Metal-based C–H activation reactions relevant in enzymatic processes
◦ Metal-organic framework (MOF)-based CO₂ reduction reactions
- 2014–2015 **Research Assistant**, CSIR-National Chemical Laboratory, India
Advisor: Prof. Debashree Ghosh
Computed ionization potentials of building-blocks of eumelanin to estimate its ionization threshold
- 2013–2014 **Master's Research**, Department of Chemistry, IITB, India
Advisor: Prof. G. Naresh Patwari
Studied unconventional hydrogen bonding in aromatic alkynes using laser and mass spectroscopy

FELLOWSHIPS AND AWARDS

- 2021 (Oct)– **Alexander von Humboldt Postdoctoral Fellowship**, MPI-P, Mainz, Germany
Present
- 2019–2020 **Doctoral Dissertation Fellowship**, University of Minnesota, MN, USA
Awarded to the University's most accomplished doctoral candidates to finalize and write their dissertation
- 2010–2014 **INSPIRE Scholar**, Department of Science and Technology, India
For being among the top 1% in higher secondary board examination
- 2012 **Dr. Sailendra Jha Memorial Prize**, R. K. M. R. College, Narendrapur, India
For appearing first class second in the university examination during bachelors study
- 2008–2012 **SSCUS Scholarship**, State Government of West Bengal, India
For academic achievements during secondary and higher secondary studies

PUBLICATIONS

- 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**, *In Press*, [doi](#) 
- Liu, J. *et al.* "Efficient and Stable Perovskite-Silicon Tandem Solar Cells Through Contact Displacement by MgF_x ." *Science* **2022**, *377*, 302. [doi](#) 
- 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](#) 
- Naujoks, T.; Jayabalan, R.; Kirsch, C.; Zu, F.; **Mandal, M.**; Wahl, J.; Waibel, M.; Andreas, O.; Koch, N.; Andrienko, D.; Scheele, M.; Brütting, W. "Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment." *ACS Appl. Mater. Interfaces* **2022**, *14*, 28985. [doi](#) 
- Lee, A. L.; Pandey, A.; Chiniforoush, 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](#) 
- Yu, X.; Fu, S.; **Mandal, M.**; Yao, X.; Liu, Z.; Zheng, W.; Samorì, P.; Narita, A.; Müllen, K.; Andrienko, D.; Bonn, M.; Wang, H. "Tuning Interfacial Charge Transfer in Atomically Precise Nanographene-Graphene Heterostructures by Engineering van der Waals Interactions." *J. Chem. Phys.* **2022**, *156*, 074702. [doi](#) 
- 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](#) 
- Wahl, J.; Engelmayer, M.; **Mandal, M.**; Naujoks, T.; Haizmann, P.; Maier, A.; Peisert, H.; Andrienko, D.; Brütting, W.; Scheele, M. "Porphyrin Functionalization of $\text{CsPbBrI}_2/\text{SiO}_2$ Core-Shell Nanocrystals Enhances the Stability and Efficiency in Electroluminescent Devices." *Adv. Optical Mater.* **2021**, 2101945. [doi](#) 
- **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](#) 
- 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](#) 
- Hu, H.; Chen, S.-J.; **Mandal, M.**; Pratik, S. M.; Buss, J. A.; Krska, S. W.; Cramer, C. J.; Stahl, S. S. "Copper-Catalyzed Benzylic C–H Coupling with Alcohols via Radical Relay Enabled by Redox Buffering." *Nat. Catal.* **2020**, *3*, 358. [doi](#) 
- Luke, A. M.; Peterson, A.; Chiniforoush, S.; **Mandal, M.**; Popowski, Y.; Sajjad, H.; Bouchey, C. J.; Shopov, D. Y.; Graziano, B. J.; Yao, L. J.; Cramer, C. J.; Reineke, T. M.; Tolman, W. B. "Mechanism of Stereocontrol in Polymerization of *rac*-Lactide by Aluminum Complexes Supported by Indolide-Imine Ligands." *Macromolecules* **2020**, *53*, 1809. [doi](#) 
- 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 $[\text{CuO}_2\text{CR}]^{2+}$ Cores." *Inorg. Chem.* **2019**, *58*, 15872. [doi](#) 
- **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](#) 
- 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](#) 
- 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](#) 
- **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](#) 
- 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](#) 
- 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](#) 

- 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](#) 
- 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](#) 
- **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](#) 

MANUSCRIPTS SUBMITTED/IN PREPARATION

- **Mandal, M.**; Buss, J. A.; Chen, S.-J.; Cramer, C. J.; Stahl, S. S. “Mechanistic studies of radical relay catalysis: Insights into radical formation and functionalization.” *In Preparation*

ORAL PRESENTATIONS

- July 2022 **Humboldt Salon (Rhein-Main region)**, Institute of Molecular Biology, Mainz, Germany
Mandal, M. “Modeling Sustainability in Chemistry: From Catalysis to Energy Materials.”
- Oct 2020 **Inorganometallic Catalyst Design Center**, All-Hands Meeting, Virtual/Zoom
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.”
- Jul 2019 **Quantum BioInorganic Chemistry Conference**, Marseille, France
Mandal, M.; Elwell, C. E.; Tolman, W. B.; Cramer, C. J. “Mechanisms for hydrogen-atom abstraction by reactive copper(III) cores: HAT or cPCET?”
- Apr 2019 **ACS National Meeting**, Orlando, FL
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.”
- Jun 2018 **Graduate Student Research Symposium**, Department of Chemistry, UMN
Mandal, M.; Cramer, C. J. “Mechanistic analysis and catalyst design for sustainable polymer synthesis.”
- May 2017 **Center for Sustainable Polymers (CSP)**, Annual Meeting, Minneapolis, MN
Mandal, M.; Dunbar, C. R.; Cramer, C. J. “Theory for mechanistic analysis and catalyst design.”

POSTER PRESENTATIONS

- Aug 2019 **Energy Frontier Research Center**, PI Meeting, Washington, D.C.
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.”
- Apr 2019 **ACS National Meeting**, Orlando, FL
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.”
- Mar 2019 **National Science Foundation**, CSP Reverse Site Visit, Alexandria, VA
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.”
- Sep 2018 **Nanoporous Materials Genome Center**, All-Hands Meeting, Minneapolis, MN
Mandal, M.; Ye, J.; Otake, K. I.; Farha, O. K.; Truhlar, D. G.; Cramer, C. J. “Computational characterization of acid functionalized metal-organic frameworks as supports for Pd(II).”
- Apr 2018 **CSP Annual Meeting**, Minneapolis, MN
Mandal, M.; Dereli, B.; Luke, A. M.; Macaranas, J. A.; Stasiw, D. E.; Tolman, W. B.; Cramer, C. J. “Computationally guided polymerization catalyst design.”

TEACHING AND OUTREACH ACTIVITIES

- 2017–2018 **Mentor**, Department of Chemistry, UMN
Mentored a high-school student | Cramer Group
- 2016–2018 **Volunteer, Minnesota State Fair**, Exhibit/Outreach
(Summer) Participated in the outreach program for three consecutive years, arranged by the Center for Sustainable Polymers to educate visitors about the benefits of bio-based polymers

- 2015–2016 **Teaching Assistant**, Department of Chemistry, UMN
Served as a teaching assistant | Undergraduate Course: General chemistry laboratory
- 2012–2013 **Teaching Assistant**, Bikrampur High School, West Bengal, India
(Summer) Taught general chemistry to high school students

References

Christopher J. Cramer

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University Teaching Professor Emeritus
Vice President for Research Emeritus
University of Minnesota
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Denis Andrienko

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