Agnes E. Thorarinsdottir

Assistant Professor of Chemistry

Department of Chemistry, University of Rochester

Email: agnes.thorarinsdottir@rochester.edu

Website: https://sas.rochester.edu/chm/groups/thorarinsdottir/

PROFESSIONAL EXPERIENCE

2023-present	Assistant Professor of Chemistry, University of Rochester, Rochester, NY, USA
2020-2023	Postdoctoral Fellow in Chemistry, Harvard University, Cambridge, MA, USA

Faculty Advisor: Daniel G. Nocera, Professor of Chemistry

<u>Project:</u> Design of Electrocatalytic Systems to Address Challenges in Energy <u>Funding:</u> Environmental Fellow, Harvard University Center for the Environment

EDUCATION

2020	Ph.l	D. in	Cl	hemistry	7, No	orthwes	stern	Unive	sity,	Evanston, I	L, USA

Faculty Advisor: T. David Harris, Assistant Professor of Chemistry

Thesis: Control of Electronic Spin in the Design of Transition Metal-Based Bioresponsive Magnetic

Resonance Imaging Probes and Metal-Organic Magnets

2015 B.S. in Chemistry, University of Iceland, Reykjavik, Iceland

Faculty Advisor: Krishna K. Damodaran, Professor of Chemistry

Thesis: Synthesis, Characterization and Catalytic Investigation of Metal-Organic Frameworks Constructed

from Salen Type Metalloligands

AWARDS & HONORS

2024-2026	Scialog Fellow for Sustainable Minerals, Metals, and Materials						
2021	ACS DIC Young Investigator Award						
2020-2022	Harvard University Center for the Environment Postdoctoral Fellow						
2020	est Poster Award, 6 th International School for Young Scientists: Magnetic Resonance and agnetic Phenomena in Chemical and Biological Physics						
2020	CAS Future Leader						
2019	Edmund W. Gelewitz Award for Excellence in Graduate Research and Service						
2019	Northwestern University Research Safety Leadership Award						
2019	WCC Merck Research Award						
2018	Donald E. Smith Teaching Award						
2017-2018	Leifur Eiriksson Foundation Scholarship						
2017	Joseph Lambert Award for Excellence in Junior Graduate Research						
2015	University of Iceland Outstanding Graduating Chemist Award						
2014	California Institute of Technology Summer Undergraduate Research Fellowship Award						

PUBLICATIONS

ORCID: 0000-0001-9378-4454; *corresponding author(s); ‡undergraduate coauthor; #equal contributions

At the University of Rochester:

24. Carmona-Pérez, D.; Gao, M.[‡]; Andes, S.[‡]; Brennessel, W. W.; **Thorarinsdottir, A. E.*** "Effect of Coordination Environment and Electronic Coupling on Redox Entropy in a Family of Dinuclear Complexes." *Under review at ACS Electrochemistry*.

- 23. Dagar, M.; De, A.; Lu, Z.; Matson, E. M.*; **Thorarinsdottir, A. E.*** "Implications of Charge and Heteroatom Dopants on the Thermodynamics and Kinetics of Redox Reactions in Keggin-Type Polyoxometalates." *ACS Mater. Au* **2025**, *5*, 200–210.
- *Prior to the University of Rochester (Postdoctoral & Graduate Research):*
- 22. Hartnett, A. C.; Evenson, R. J.; **Thorarinsdottir, A. E.**; Veroneau, S. S.; Nocera, D. G.* "Lanthanum-Promoted Electrocatalyst for the Oxygen Evolution Reaction: Unique Catalyst or Oxide Deconstruction?" *J. Am. Chem. Soc.* **2025**, 147, 1123–1133.
- 21. Li, Y.; Stec, G. J.; **Thorarinsdottir, A. E.**; McGillicuddy, R. D.; Zheng, S.-L.; Mason, J. A.* "The Role of Metal Accessibility on Carbon Dioxide Electroreduction in Atomically Precise Nanoclusters." *Chem. Sci.* **2023**, *14*, 12283–12291.
- 20. Yan, Z.; Reynolds, K. G.; Sun, R.; Shin, Y.; **Thorarinsdottir, A. E.**; Gonzalez, M. I.; Kudisch, B.; Galli, G.; Nocera, D. G.* "Oxidation Chemistry of Bicarbonate and Peroxybicarbonate: Implications for Carbonate Management in Energy Storage." *J. Am. Chem. Soc.* **2023**, *145*, 22213–22221.
- 19. **Thorarinsdottir, A. E.***; Erdosy, D. P.*; Costentin, C.*; Mason, J. A.*; Nocera, D. G.* "Enhanced Activity for the Oxygen Reduction Reaction in Microporous Water." *Nat. Catal.* **2023**, *6*, 425–434.
- 18. Veroneau, S. S.; **Thorarinsdottir, A. E.**; Loh, D. M.; Hartnett, A. C.; Keane, T. P.; Nocera, D. G.* "Electrolyte-Induced Restructuring of Acid-Stable Oxygen Evolution Catalysts." *Chem. Mater.* **2023**, *35*, 3218–3225.
- 17. Nava, M.; **Thorarinsdottir, A. E.**; Lopez, N.; Cummins, C. C.*; Nocera, D. G.* "Chemical Challenges that the Peroxide Dianion Presents to Rechargeable Lithium—Air Batteries." *Chem. Mater.* **2022**, *34*, 3883–3892 (invited article for Virtual Special Issue, "John Goodenough at 100").
- 16. Veroneau, S. S.; Hartnett, A. C.; **Thorarinsdottir, A. E.**; Nocera, D. G.* "Direct Seawater Splitting by Forward Osmosis Coupled to Water Electrolysis." *ACS Appl. Energy Mater.* **2022**, *5*, 1403–1408.
- 15. **Thorarinsdottir**, **A. E.***; Veroneau, S. S.*; Nocera, D. G.* "Self-Healing Oxygen Evolution Catalysts." *Nat. Commun.* **2022**, *13*, 1243 (invited article).
- 14. **Thorarinsdottir, A. E.**; Costentin, C.; Veroneau, S. S.; Nocera, D. G.* "p-Block Metal Oxide Noninnocence in the Oxygen Evolution Reaction in Acid: The Case of Bismuth Oxide." *Chem. Mater.* **2022**, *34*, 826–835.
- 13. Wang, Y.; Ziebel, M. E.; Sun, L.; Gish, J. T.; Pearson, T. J.; Lu, X.-Z.; **Thorarinsdottir, A. E.**; Hersam, M. C.; Long, J. R.*; Freedman, D. E.*; Rondinelli, J. M.*; Puggioni, D.*; Harris, T. D.* "Strong Magnetocrystalline Anisotropy Arising from Metal–Ligand Covalency in a Metal–Organic Candidate for 2D Magnetic Order." *Chem. Mater.* **2021**, *33*, 8712–8721.
- 12. **Thorarinsdottir, A. E.**; Nocera, D. G.* "Energy Catalysis Needs Ligands with High Oxidative Stability." *Chem Catal.* **2021**, *1*, 32–43 (invited article for Inaugural Issue).
- 11. Margarit, C. G.; Asimow, N. G.; **Thorarinsdottir, A. E.**; Costentin, C.*; Nocera, D. G.* "Impactful Role of Cocatalysts on Molecular Electrocatalytic Hydrogen Production." *ACS Catal.* **2021**, *11*, 4561–4567.
- 10. **Thorarinsdottir, A. E.**; Bjornsson, R.; Harris, T. D.* "Insensitivity of Magnetic Coupling to Ligand Substitution in a Series of Tetraoxolene Radical-Bridged Fe₂ Complexes." *Inorg. Chem.* **2020**, *59*, 4634–4649.
- 9. **Thorarinsdottir, A. E.**; Harris, T. D.* "Metal–Organic Framework Magnets." *Chem. Rev.* **2020**, *120*, 8716–8789 (invited article for Thematic Issue, "Porous Framework Chemistry").
- 8. Wang, X.; **Thorarinsdottir, A. E.**; Bachrach, M.; Blayney, M. B.* "Building a Sustainable Student-Led Model to Promote Research Safety in Academic Laboratories." *ACS Cent. Sci.* **2019**, *5*, 1900–1903.
- Valdez-Moreira, J. A.; Thorarinsdottir, A. E.; DeGayner, J. A.; Lutz, S. A.; Chen, C.-H.; Losovyj, Y.; Pink, M.; Harris, T. D.*; Smith, J. M.* "Strong π-Backbonding Enables Record Magnetic Exchange Coupling Through Cyanide." *J. Am. Chem. Soc.* 2019, 141, 17092–17097.
- 6. Du, K.; **Thorarinsdottir, A. E.**; Harris, T. D.* "Selective Binding and Quantitation of Calcium with a Cobalt-Based Magnetic Resonance Probe." *J. Am. Chem. Soc.* **2019**, *141*, 7163–7172.
- 5. **Thorarinsdottir, A. E.**; Harris, T. D.* "Dramatic Enhancement in pH Sensitivity and Signal Intensity Through Ligand Modification of a Dicobalt PARACEST Probe." *Chem. Commun.* **2019**, *55*, 794–797.

- 4. **Thorarinsdottir, A. E.**; Tatro, S. M.[‡]; Harris, T. D.* "Electronic Effects of Ligand Substitution in a Family of Co^{II}₂ PARACEST pH Probes." *Inorg. Chem.* **2018**, *57*, 11252–11263.
- 3. Gaudette, A. I.; **Thorarinsdottir, A. E.**; Harris, T. D.* "pH-Dependent Spin State Population and ¹⁹F NMR Chemical Shift via Remote Ligand Protonation in an Iron(II) Complex." *Chem. Commun.* **2017**, *53*, 12962–12965.
- 2. **Thorarinsdottir, A. E.**; Du, K.; Collins, J. H. P.; Harris, T. D.* "Ratiometric pH Imaging with a Co^{II}₂ MRI Probe via CEST Effects of Opposing pH Dependences." *J. Am. Chem. Soc.* **2017**, *139*, 15836–15847.
- 1. **Thorarinsdottir, A. E.**; Gaudette, A. I.; Harris, T. D.* "Spin-Crossover and High-Spin Iron(II) Complexes as Chemical Shift ¹⁹F Magnetic Resonance Thermometers." *Chem. Sci.* **2017**, *8*, 2448–2456.

PRESENTATIONS

Invited Presentations

At the University of Rochester:

- University of Buffalo, Department of Civil, Structural & Environmental Engineering Seminar Series, Buffalo, NY, April 2025
 - Title: "Advancing Electrochemical Properties via Synthetic Design"
- Pittcon Conference & Exposition, Boston, MA, March 2025
 Title: "Harnessing Porous Frameworks for Controlling Electrocatalyst Microenvironments"
- University of Rochester, Materials Research Society, Rochester, NY, September 2023
 Title: "The Thorarinsdottir Research Group: Advancing Electrochemical Properties via Synthetic Design"

Prior to the University of Rochester:

- Northwestern University, Safety Awareness Week, Keynote Speaker, Evanston, IL, April 2023 Title: "How RSSI Started and Importance of Research Safety"
- Washington University, St. Louis, Chemistry Seminar Series, St. Louis, MO, February 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Colorado, Boulder, RASEI Institute Seminar Series, Boulder, CO, February 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- Dartmouth College, Chemistry Seminar Series, Hanover, NH, February 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Virginia, Chemistry Seminar Series, Charlotte, VA, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Florida, Chemistry Seminar Series, Gainesville, FL, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of California, Los Angeles, Chemistry and Biochemistry Seminar Series, Los Angeles, CA, January 2023 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Rochester, Chemistry Seminar Series, Rochester, NY, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- **Purdue University**, Chemistry Seminar Series, West Lafayette, IN, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- Cornell University, Chemistry and Chemical Biology Seminar Series, Ithaca, NY, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- Florida State University, Chemistry and Biochemistry Seminar Series, Tallahassee, FL, January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- Georgetown University, Chemistry Seminar Series, Washington D.C., January 2023
 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Iceland, Chemistry and Biochemistry Seminar Series, Reykjavik, Iceland, January 2023 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"

- University of Indiana, Bloomington, Chemistry Seminar Series, Bloomington, IN, December 2022 Title: "New Approaches to Magnetic Resonance Imaging and Energy Catalysis Through Chemical Design"
- University of Chicago, Future Faculty Symposium, May 2022
 Title: "Electrocatalytic Oxygen Evolution Reaction in Acid Using Earth Abundant Elements: The Case of Bismuth Oxide"
- ACS National Meeting, Inorganic Young Investigator Awards Session, Virtual, August 2021
 Title: "Control of Electronic Spin in the Design of Transition Metal-Based Bioresponsive Magnetic Resonance Imaging Probes"
- ACS National Meeting, WCC Merck Research Awards Symposium, San Diego, CA, August 2019 Title: "Ratiometric Imaging of pH with Dicobalt PARACEST MRI Probes"

Other Conference Participation Prior to the University of Rochester

- Inorganic Chemistry GRS & GRC, Newport, RI, May–June 2022
 Title of poster: "Strategies Toward Increased Energy and Carbon Efficiency in Low-Temperature CO₂ Electrolysis"
- Solar Fuels GRS & GRC, Lucca, RI, May 2022
 Title of poster: "Strategies Toward Increased Energy and Carbon Efficiency in Low-Temperature CO₂ Electrolysis"
- ACS National Meeting, San Diego, CA, March 2022
 Title of talk: "p-Block Metal Oxide Noninnocence in the Oxygen Evolution Reaction in Acid"
- Harvard University Chemistry and Chemical Biology Research Symposium, Virtual, May 2021 Title of talk: "Main Group Metal Oxides as Oxygen Evolution Reaction Catalysts in Acid"
- 6th International School for Young Scientists: Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics, Virtual, September 2020

 Title of talk: "Control of Electronic Spin in the Design of Transition Metal-Based Rioresponsive Magnetic Resonance

Title of talk: "Control of Electronic Spin in the Design of Transition Metal-Based Bioresponsive Magnetic Resonance Imaging Probes"

- **ACS National Meeting**, San Diego, CA, August 2019
 Title of talk: "Fe^{II} Spin-Crossover Complexes as Temperature- and pH-Responsive ¹⁹F Chemical Shift Magnetic Resonance Probes"
- Imaging in 2020, Grand Teton National Park, WY, September 2018
 Title of poster: "Quantitation of pH and Temperature with Transition Metal Complexes via Magnetic Resonance Imaging"
- Inorganic Chemistry GRS & GRC, Biddeford, ME, June 2018
 Title of poster: "Quantitation of pH and Temperature with Transition Metal Complexes via Magnetic Resonance Imaging"
- Hazard and Risk Management in the Laboratory Laboratory Safety Workshop, Chicago, IL, May 2018
 Title of poster: "Graduate Student Led Safety Team: An Approach to Engage Researchers in Laboratory Safety"

MENTORED RESEARCHERS

Current Group: 1 postdoctoral researcher, 4 Ph.D. students, and 5 B.S./B.A. students

Present: Azina Rahmani (postdoc); Anyesh De (G2); Daniela Carmona Perez (G2); Phillip Dinga (G2); Qishen Lyu (G2); Bryce Kneer (U4); James Kim (U4); Jonathan Pulido (U2); Steven Riera (U4); Yuanxi Gao (U3)

Alumni: Meiqin Gao (B.A., 2024); Samantha Andes (REU, 2024); Duong Minh Truong (i-Scholar, 2023)

SYNERGISTIC ACTIVITIES & SERVICE

Teaching Activities

At the University of Rochester:

• Physical Methods in Inorganic Chemistry (CHEM 426), Spring 2025 (4 credit hours)

- Organometallic Chemistry (CHEM 421), Fall 2024 (2 credit hours)
- Guest Lecturer, Inorganic Chemistry, Chapman University, Spring 2024 (Virtual)
- Group Theory (CHEM 415), Fall 2023, 2024 (2 credit hours)
- Physical Methods in Inorganic Chemistry (CHEM 424), Fall 2023 (2 credit hours)

Prior to the University of Rochester:

- Introductory Inorganic Chemistry (CHEM 40), Spring 2021, Harvard University (Head TA)
- Advanced Inorganic Chemistry (CHEM 435), Winter 2018 & 2019, Northwestern University (Head TA)
- General Chemistry (CHEM 101), Fall 2016, Northwestern University (TA)
- Organic Chemistry Laboratory (CHEM 232), 2015–2016, Northwestern University (TA)

National & International Activities

- Guest Editor, JoVE, Methods Collection: Electrochemical Methods in Energy Catalysis (2024–present)
- Mentor, Chemistry Women Mentorship Network (Chem WMN) (2023–present)
- Guest Editor, Special Issue of Supramolecular Chemistry for ISMSC 2023 (2023–2024)
- Organizing Committee Member, 17th International Symposium on Macrocyclic and Supramolecular Chemistry (2023)
- Oral & Poster Presentation Referee, Western New York Inorganic Chemistry Symposium (2023)

Reviewing Activities

National Science Foundation (NSF) (2024–present)

Science Foundation of Ireland (2024)

Journals: ACS Applied Nano Materials, ACS Catalysis, ACS Omega, Acta Crystallographica, ChemCatChem, Chemical Communications, Chemical Science, Chemistry of Materials, Inorganic Chemistry Frontiers, Journal of the American Chemical Society, Nature Catalysis

Professional Affiliations

- American Chemical Society, Division of Inorganic Chemistry (2020–present)
- American Chemical Society (2019–present)
- Phi Lambda Upsilon Graduate Chemistry Honor Society (2017–present)
- Icelandic Chemical Society (2015–present)

Service & Outreach Activities

At the University of Rochester:

- University of Rochester, Sproull Fellowship Committee Chair (February 2025)
- University of Rochester, Chemistry DEIO: Events & Forums Subcommittee Member (2024–present)
- University of Rochester, Upward Bound Pre-College Program Course Instructor (2024–present)
- University of Rochester, Chemistry Graduate Studies Committee Member (2024–present)
- University of Rochester, Graduate Research Symposium Poster Referee (April 2024)
- University of Rochester, Schwartz Discover Grant Reviewer (April 2024)
- University of Rochester, Hooker Dissertation Fellowship Committee Member (April 2024)
- University of Rochester, LEAP Program Career Day Volunteer (March 2024)
- University of Rochester, Data Bloom Referee (January 2024)
- University of Rochester, National Chemistry Week Volunteer (2023–present)
- University of Rochester, Chemistry Graduate Student Admissions Committee Member (2023–present)
- University of Rochester, Materials Science Graduate Student Admissions Committee Member (2023–present)
- University of Rochester, Chemistry DEIO: Community Engagement Subcommittee Member (2023–present)

Prior to the University of Rochester:

- Harvard University, Harvard University Women+ in Chemistry, Executive Board Member (2021–2023)
- Science Club for Girls, Cambridge, MA, Volunteer (2021–2023)
- Harvard University, Department of Chemistry & Chemical Biology, Peer Mentor (2021–2023)
- Harvard University, Department of Chemistry & Chemical Biology, SACNAS Conference Rep. (October 2021)

- Northwestern University, Career Day for Girls, Group Leader (February 2019)
- Northwestern University, Department of Chemistry, Graduate Recruitment Focus Group Member (2018–2019)
- Northwestern University, Department of Chemistry, Peer Mentor (2018–2019)
- Northwestern University, Phi Lambda Upsilon, Alpha Gamma Chapter, President (2018–2019)
- Northwestern University, EPIC Cleanup Day, Organizer (October 2018)
- Northwestern University, Phi Lambda Upsilon, Alpha Gamma Chapter, Secretary (2017–2018)
- Northwestern University, Sports & STEM Program, Group Leader (2017–2018)
- Northwestern University, Research Safety Student Initiative, Co-Founder & Vice President (2017–2019)
- Northwestern University, International Summer Institute, Volunteer (2017–2019)
- Northwestern University, Science in the Classroom Outreach Program, Group Leader (2016–2019)
- Northwestern University, Department of Chemistry, Teaching Assistant Training, Co-Organizer (2016–2019)

Professional Development Activities

- University of Rochester, "NSF CAREER Bootcamp" Workshop Series (May 2024–June 2024)
- University of Rochester, "Supporting Undergraduate Students in Summer Research" Workshop (May 2024)
- University of Rochester, "Trauma-Informed Conversations" Workshop (April 2024)
- University of Rochester, "Navigating Difficult Conversations in Graduate Mentoring" Workshop (March 2024)
- University of Rochester, "Intercultural Communication" Workshop (November 2023)
- University of Rochester, "Effective Study Strategies for Students" Workshop (October 2023)
- University of Rochester, Inclusive STEM Teaching Group (September 2023–November 2023)
- University of Rochester, Active Learning Teaching Group (September 2023–November 2023)