

Contact Information

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Areas of Expertise

- Physical chemistry | Theoretical chemistry
- Computational chemistry | Electronic structure calculations | Multiscale modeling | Enzymatic catalysis | Photochemistry | Vitamin B₁₂ chemistry, photochemistry, & enzymology | Photoreceptor proteins |

Current Position

Department of Chemistry
University of Louisville
Louisville, Kentucky

January 2024-present

✓ **Postdoctoral Scholar**

- Advisor: Prof. Lee Thompson

Project: Dynamic correlation of nonorthogonal CI methods

Previous Postdoctoral Position

Fritz Haber Center for Molecular Dynamics
The Hebrew University of Jerusalem
Jerusalem, Israel

2021-2023

✓ **Zuckerman STEM Leadership Program Postdoctoral Scholar**

- Advisor: Prof. Igor Schapiro
- Project: Rational Design of Red-Shifted Photoreceptor Proteins for Biotechnological Applications via Multiscale Modelling

Education

Graduate Level

Department of Chemistry, University of Louisville
Louisville, Kentucky, U.S.A.

2016-2021

✓ **PhD, Physical Chemistry**

✓ **MS, Physical Chemistry**

- Thesis Advisor: Prof. Pawel M. Kozlowski
- Thesis: *Computational Investigations of the Photochemical Properties of B₁₂-Dependent Systems: From Solution to Enzymes*
- University of Louisville School of Interdisciplinary and Graduate Studies University Fellow

Department of Chemistry, University of Louisville

2018-2021

✓ **Graduate Teaching Assistant**

Taught quantum chemistry recitation, general chemistry recitation, general chemistry laboratories, and honors laboratory courses with a teaching load of 5 courses per semester with ~20 students per class

Course Load:

CHM 101, Grading Proctor

- Fall 2021

CHM 202, General Chemistry II – Recitation (Lecture style, virtual format)

- Summer 2021
- 25 students

CHM 207, Head Teaching Assistant, Intro to Chemistry Analysis I – Laboratory

- Spring 2021

CHM 207, Intro to Chemical Analysis I – Laboratory

- Fall 2018, Spring 2019, Fall 2020, Spring 2021, Fall 2021
- 3-5 sections per semester, 20 students per section

CHM 208, Intro to Chemical Analysis II – Laboratory

- Spring 2020, Fall 2020, Spring 2021
- 3 Sections per semester, 20 students per section

CHM 207, Honors Intro to Chemical Analysis I – Laboratory

- Fall 2020, Fall 2021
- 2 sections per semester, 20 students per section

CHM 208, Honors Intro to Chemical Analysis II – Laboratory

- Fall 2020, Fall 2021
- 3 sections per semester, 20 students per section

CHM 209, Intro to Chemical Analysis III – Laboratory

- Spring 2020, Spring 2021
- 2 sections per semester, 15 students per section

CHM 441, Elements of Physical Chemistry – Recitation (Lecture style)

- Fall 2020
- 1 section, 25 students

CHM 465, Physical Chemical I, Quantum Mechanics – Recitation (Lecture style)

- Fall 2018
- 1 section, 35 students

Research mentor for undergraduate research student

- Spring 2017

Department of Chemistry, University of Louisville

- ✓ **President, Chemistry Graduate Student Association**

2018-2020

- Planned events for graduate students - welcome picnic for new graduate students, career information panel with University of Louisville Chemistry PhD program alumni, and Derby Lecture Series
- Organized **41st Annual Derby Lecture Series** (May 2 and 3 2019) featuring the **2016 Nobel Laureate, Sir J. Fraser Stoddart**
- Organized **42nd Annual Derby Lecture Series** (postponed due to COVID-19 until May 2022) featuring the **2019 Nobel Laureate, M. Stanly Whittingham**
- Oversaw fundraising efforts and acquired university and corporate funding
 - Fundraising: \$13,048.13
 - University of Louisville Club Program Committee Grants: \$1,200.00
 - Corporate Sponsorships: \$14,000.00

- Acted as a liaison between chemistry graduate students and the graduate student council, provided council for success in graduate school to new graduate students, lead campus tours for prospective graduate students
- Served as graduate student representative on the Chemistry Department Advisory Board

Undergraduate Level

Department of Chemistry, Misericordia University
Dallas, Pennsylvania, U.S.A

2012-2015

✓ **BS in Chemistry,**
Magna Cum Laude

✓ **Minor in Mathematics**

Misericordia University

2013-2015

✓ **Student Researcher**

- Misericordia University Summer Undergraduate Research Fellowship Program (SURF)
- Advisor: Prof. Anna Fedor
- Research Project: Computational investigations of the self-association of phenols

✓ **Work Study: Laboratory Assistant**

- Advisor: Leo Carr
- Assisted the laboratory manager in the set-up/take-down of undergraduate laboratories including introductory and advanced chemistry and biology laboratories
- Responsible for organization and management of chemical and glassware stockrooms and proper disposal of waste
- Prepared solutions and reagents for laboratory sections

Department of Chemistry, North Carolina State University
Raleigh, North Carolina, U.S.A.

Summer 2015

✓ **Research Fellow**

- National Science Foundation Research Experience for Undergraduates Program (REU)
- Advisor: Prof. Felix N. Castellano
- Research Project: Photochemical investigations of copper bis-phenanthroline compounds

Other Work Experience

Quality Assurance Chemist, American Synthetic Rubber Company
Louisville, Kentucky, U.S.A

Feb 2016-Jul 2016

Teller and Customer Service Representative, People's Security Bank and Trust Co.
Scranton, Pennsylvania, U.S.A

Jan 2009-Dec 2015

Publications

- Mackintosh, M.J.,** Hoischen, D., Dieter, H-D, Schapiro, I. Gäertner, W. Merocyanines form Bacteriorhodopsins with Strongly Bathochromic Absorption Maxima. *J. Photochem. Photobiol.* **2023**. <https://doi.org/10.1007/s43630-023-00496-0>
- Sukhran, Y., Alshanski, I., Filiba, O., **Mackintosh, M.J.,** Schapiro, I., Hurevich, M. Unexpected Nucleophile Masking in Acyl Transfer to Sterically Crowded and Conformationally Restricted Galactosides. *J. Org. Chem.* **2023**, 88, 9313–9320.
- Phipps, C.A., Hofsommer, D.T., **Toda, M.J.,** Nkurunziza, F., Shah, B., Spurgeon, J.M., Kozlowski, P.M., Buchanan, R.M., Grapperhaus, C.A. Ligand-Centered Hydrogen Evolution with Ni(II) and Pd(II)DMTH. *Inorg. Chem.* **2022**, 61, 25, 9792–9800.

20. **Toda, M.J.**, Lodowski, P., Mamun, A.A., Kozlowski, P.M. Photoproduct formation in coenzyme B₁₂-dependent CarH via a singlet pathway. *J. Photochem. Photobiol. B: Biol.* **2022**, 232, 112471.
19. **Toda, M.J.**, Ghosh, A.P., Parmar, S., Kozlowski, P.M. Computational Investigations of B₁₂-Dependent Enzymatic Reactions. **In Book:** "B₁₂ Enzymes" in series *Methods in Enzymology*. **2022**, Vol. 667. Ed. Neil Marsh.
18. Ghosh, A. P., **Toda, M.J.**, Kozlowski, P.M. Photolytic Properties of B₁₂-Dependent Enzymes: A Theoretical Perspective. **In Book:** "Vitamin B₁₂" in series *Vitamins and Hormones*. **2022**, Ed. Gerald Litwak.
17. **Toda, M.J.**, Lodowski, P., Mamun, A.A., Kozlowski, P.M. Electronic and Photolytic Properties of Hydridocobalamin. *J. Photochem. Photobiol. B: Biol.* **2021**, 224, 112295.
16. Ghosh, A. P., **Toda, M. J.**, Kozlowski, P.M. What Triggers the Cleavage of the Co-C₅ Bond in Coenzyme B₁₂-Dependent Itaconyl-CoA Methylmalonyl-CoA Mutase? *ACS Catal.* **2021**, 11, 7943-7955.
15. **Toda, M. J.**, Lodowski, P., Thurman, T. M., Kozlowski, P. M. Light Mediated Properties of a Thiolato-derivative of Vitamin B₁₂. *Inorg. Chem.* **2020**, 59, 17200-17212.
14. **Toda, M. J.**, Mamun, A. A., Lodowski, P. Kozlowski, P. M. Why is CarH Photolytically Active in Comparison to other B₁₂-dependent Enzymes? *J. Photochem. Photobiol. B: Biol.* **2020**, 111919.
13. Cronin, S. P., Mamun, A. A., **Toda, M. J.**, Mashuta, M. S., Losovyj, Y., Kozlowski, P. M., Buchanan, R. M., Grapperhaus, C. A. Utilizing Charge Effects and Minimizing Intramolecular Proton Rearrangement to Improve the Overpotential of a Thiosemicarbazonato Zinc HER Catalyst. *Inorg. Chem.* **2019**, 58, 12986-12997.
12. Michocki, L. B.; Miller, N. A.; Alonso-Mori, R.; Britz, A.; Deb, A.; Glownia, J. M.; Kaneshiro, A. K.; Konar, A.; Koralek, J.; Meadows, J. H.; Sofferman, D. L.; Song, S.; **Toda, M. J.**; van Driel, T. B.; Kozlowski, P. M.; Kubarych, K. J.; Penner-Hahn, J. E.; Sension, R. J. Probing the Excited State of Methylcobalamin Using Polarized Time-Resolved X-ray Absorption Spectroscopy. *J. Phys. Chem. B* **2019**, 123, 6042-6048.
11. Mamun, A. A., **Toda, M. J.**, Lodowski, P., Kozlowski, P. M. Photolytic Cleavage of Co-C Bond in Coenzyme B₁₂-Dependent Glutamate Mutase. *J. Phys. Chem. B* **2019**, 12, 2585-2598.
10. **Toda, M. J.**, Lodowski, P., Mamun, A. A., Jaworska, M., Kozlowski, P. M. Photolytic Properties of the Biologically Active Forms of Vitamin B₁₂. *Coord. Chem. Rev.* **2019**, 385, 20-43.
9. Mamun, A. A., **Toda, M. J.**, Kozlowski, P. M. Can Photolysis of the Co-C Bond in Coenzyme B₁₂-dependent Enzymes be used to Mimic the Native Reaction? *J. Photochem. Photobio. B: Bio.* **2019**, 191, 175-184.
8. **Toda, M. J.**, Kozlowski, P. M., Andruniow, T. Assessing Electronically Excited States of Cobalamins via Absorption Spectroscopy and Time-Dependent Density Functional Theory. **In book:** *Transition Metals in Coordination Environments: Computational Chemistry and Catalysis Viewpoints*. Springer. **2019**, Chapter 8, Pages 219-258. DOI: 10.1007/978-3-030-11714-6_8.
7. Wiley, T. E., Miller, N. A., Miller, W. R., Sofferman, D. L., Lodowski, P., **Toda, M. J.**, Jaworska, M., Kozlowski, P. M., and Sension, R. J. Off to the Races: Comparison of Excited State Dynamics in Vitamin B₁₂ Derivatives Hydroxocobalamin and Aquocobalamin. *J. Phys. Chem. A* **2018**, 122, 6693-6703.
6. Lodowski, P., **Toda, M. J.**, Ciura, K., Jaworska, M., Kozlowski, P. M. Photolytic Properties of Antivitamins B₁₂. *Inorg. Chem.* **2018**, 57, 7838-7850.
5. Mamun, A. A., **Toda, M. J.** Lodowski, P., Jaworska, M., Kozlowski, P. M. Mechanism of Light Induced Radical Pair Formation in Coenzyme B₁₂-Dependent Ethanolamine Ammonia-Lyase. *ACS Catalysis.* **2018**, 8, 7164-7178.
4. Miller, N. A., Deb, A., Alonso-Mori, R., Glownia, J. M., Kiefer, L. M., Konar, A., Michocki, L. B., Sikorski, M., Sofferman, D. L., Song, S., **Toda, M. J.**, Wiley, T. E., Zhu, D., Kozlowski, P. M., Kubarych, K. J., Penner-Hahn, J. E., Sension, R. J. Ultrafast X-ray Absorption Near Edge Structure Reveals Ballistic Excited State Structural Dynamics. *J. Phys. Chem. A* **2018**, 122, 4963-4971.
3. Fedor, A. M., **Toda, M. J.** Applying Intermolecular Hydrogen Bonding Interactions of Phenol Derivatives to the Harmonic Oscillator Using Infrared Spectroscopy. *Chem. Ed.* **2018**, 23, 133-136.

2. Lodowski, P., Ciura, K., **Toda, M. J.**, Jaworska, M., Kozlowski, P. M. Photodissociation of Ethylphenylcobalamin Antivitamin B₁₂. *Phys. Chem. Chem. Phys.* **2017**, 19, 30310-30315.
1. Fedor, A. M., **Toda, M. J.** Investigating Hydrogen Bonding in Phenol using Infrared Spectroscopy and Computational Chemistry. *J. Chem. Ed.* **2014**, 91, 2191-2194.

Book Chapters & Reviews:

19. **Toda, M.J.**, Ghosh, A.P., Parmar, S., Kozlowski, P.M. Computational Investigations of B₁₂-Dependent Enzymatic Reactions. **In Book:** "B₁₂ Enzymes" in series *Methods in Enzymology*. **2022**, Vol. 667. Ed. Neil Marsh.
18. Ghosh, A. P., **Toda, M.J.**, Kozlowski, P.M. Photolytic Properties of B₁₂-Dependent Enzymes: A Theoretical Perspective. **In Book:** "Vitamin B₁₂" in series *Vitamins and Hormones*. **2022**, Ed. Gerald Litwak.
10. **Toda, M. J.**, Lodowski, P., Mamun, A. A., Jaworska, M., Kozlowski, P. M. Photolytic Properties of the Biologically Active Forms of Vitamin B₁₂. *Coord. Chem. Rev.* **2019**, 385, 20-43.
8. **Toda, M. J.**, Kozlowski, P. M., Andruniow, T. Assessing Electronically Excited States of Cobalamins via Absorption Spectroscopy and Time-Dependent Density Functional Theory. **In book:** *Transition Metals in Coordination Environments: Computational Chemistry and Catalysis Viewpoints*. Springer. **2019**, Chapter 8, Pages 219-258. DOI: 10.1007/978-3-030-11714-6_8.

Presentations

9. **Mackintosh, M. J.**, Schapiro, I. Strategies for far-red shifted absorption in retinal proteins. 4th Israeli Conference on Computational Modeling of Molecules and Solids. Jerusalem, Israel. July **2023**.
8. **Mackintosh, M. J.**, Schapiro, I. Strategies for far-red shifted absorption in retinal proteins. 19th International Conference on Retinal Proteins. Sapporo, Japan. Oct. **2022**.
7. **Toda, M. J.**, Mamun, A. A., Ghosh, A. P., Kozlowski, P.M. Comparison of the Photolytic Properties of B₁₂-dependent Enzymes. SERMACS, Augusta, GA. Physical Chemistry Division Poster Session. Nov. **2018**.
6. **Toda, M. J.**, Lodowski, P., Ciura, K., Jaworska, M., Kozlowski, P. M. Photochemical Properties of Vitamin B₁₂ Derivatives: Implications from TD-DFT Calculations. American Chemical Society National Meeting, New Orleans, LA. Computers in Chemistry Division Poster Session, **2018**.
5. **Toda, M. J.**, Lodowski, P., Ciura, K., Jaworska, M., Kozlowski, P. M. Photochemical Properties of Vitamin B₁₂ Derivatives: Implications from TD-DFT Calculations. Graduate Student Regional Research Conference. University of Louisville, **2018**.
4. **Toda, M. J.**, McCusker, C., Castellano, F. N. Excited State Properties of Copper(I) *bis*-Phenanthroline Complexes. Council of Undergraduate Research's REU Symposium. NSF, Alexandria, VA, **2015**.
3. **Toda, M. J.**, McCusker, C., Castellano, F. N. Excited State Properties of Copper(I) *bis*-Phenanthroline Complexes. Undergraduate Research Symposium. North Carolina State University, Raleigh, North Carolina, **2015**.
2. Fedor, A. M. and **Toda, M. J.** Examining the Intermolecular Interactions of Ionic Liquids and Phenol Derivatives using Far-Infrared Spectroscopy and Computational Chemistry. American Chemical Society National Meeting, Boston, MA, **2015**.
1. **Toda, M. J.** and Fedor, A. M. Analysis of the Intermolecular Hydrogen Bonding Interactions of Phenol Derivatives in Solution using Infrared Spectroscopy and Density Functional Theory. American Chemical Society National Meeting, Boston, MA, **2015**.

Continuing Education

The M2D School, Universidad Autónoma de Madrid
Madrid, Spain

November 2022

School on High-Performance Multilayer Molecular Dynamics Approaches

Awards

University of Louisville

- School of Interdisciplinary and Graduate Studies Univ. Fellowship *2016-2018*
- Graduate Network in Arts and Sciences Travel Award *Fall 2018*
- Graduate Student Council Travel Award *Fall 2018*
- Graduate Student Council Travel Award *Spring 2018*

Misericordia University

- Presidential Scholarship *2012-2015*
- Mission Award *2012-2015*