

# Tina N. Mihm

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## Education

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Aug 2017 – Present	<p>PhD in Chemistry, <b>University of Iowa</b>, Iowa City, IA</p> <ul style="list-style-type: none"><li>Degree expected August 2022</li><li>Thesis title: “Developing Methods to Accelerate Convergence to the Thermodynamic Limit for Periodic Coupled Cluster Theory”</li><li>Advisor: Prof. James J. Shepherd</li></ul>
Jan 2014 – May 2017	<p>B.A. in Chemistry, <b>Carthage College</b>, Kenosha, WI</p> <ul style="list-style-type: none"><li>Minor: Secondary Education (Grades 6-12)</li><li>GPA: 3.71/4.0, Dean’s list 7 semesters</li><li>Honors: Magna Cum Laude</li></ul>
Aug 2011 – Dec 2013	<p>A.S., <b>McHenry County College</b>, Crystal Lake, IL</p> <ul style="list-style-type: none"><li>GPA: 3.93/4.0</li><li>Honors: High Honors</li></ul>

## Research Experience

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Aug 2017 – Present	<p><i>Graduate Research Assistant</i>, <b>University of Iowa</b>   Shepherd Group</p> <ul style="list-style-type: none"><li>Used an in-group FORTRAN-based coupled cluster code to develop a new cost-saving, twist-averaging algorithm call connectivity twist-averaging (cTA) for use with the UEG model system</li><li>Used our new cTA code to study the convergence rates of the finite size effects in the correlation energy of metals using the UEG as a model system</li><li>Used initiator full configuration interaction quantum Monte Carlo (<i>i</i>-FCIQMC) to demonstrate a successful transfer of the cTA algorithm to quantum Monte Carlo methods</li><li>Develop a second cost-saving method for use with real solids using the transition structure factor found in the correlation energy of solids called structure factor twist averaging (sfTA)</li><li>Worked in collaboration with Dr. Andreas Grüneis, Vienna University of Technology, to develop our new sfTA for integration with the Vienna Ab initio Simulation Package (VASP)</li><li>Applied our new sfTA algorithm to coupled cluster to study properties of metals, including calculating the transition pressure of two phases of silicon</li></ul>
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## Selected Research Awards and Honors

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July 2020	<p><b>Outstanding Graduate Student Poster</b>, Virtual Conference on Theoretical Chemistry 2020 Awarded for exceptional virtual lightning talk/poster on research</p>
Feb 2020 – May 2020	<p><b>Graduate College Post-Comprehensive Research Fellowship</b>, University of Iowa Awarded for distinguished academic achievement during early graduate training</p>
April 2019	<p><b>Dr. Eunice Schuytema Beam Travel Grant</b>, University of Iowa Awarded by Women in Science and Engineering for presenting selected research at a national conference</p>

## Teaching Experience

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Jan 2019 – present	<p><i>Undergraduate Research Mentor, University of Iowa, Iowa City, IA</i></p> <ul style="list-style-type: none"><li>• Mentored three undergraduate students as they worked on various research projects in the Shepherd group centered around solid-state work</li><li>• Mentored and worked with a student on a project focused on writing Python-based POGIL style worksheet to introduce students to programming through Chemistry</li></ul>
Aug 2018 – Dec 2018	<p><i>Teaching Assistant – Physical Chemistry II, University of Iowa, Iowa City, IA</i></p> <ul style="list-style-type: none"><li>• Assisted in instruction for a POGIL based Quantum Chemistry class</li><li>• Developed/ ran active learning-based discussions</li></ul>
Aug 2017 – May 2018	<p><i>Teaching Assistant – Principles of Chemistry I Lab, University of Iowa, Iowa City, IA</i></p> <ul style="list-style-type: none"><li>• Demonstrated and instructed students in good lab practices</li><li>• Instructed students in introductory Chemistry labs</li></ul>
Spring 2017	<p><i>Student Teacher, Lakeview Technology Academy, Pleasant Prairie, WI</i></p> <ul style="list-style-type: none"><li>• Taught 10<sup>th</sup> grade Chemistry classes for half a semester</li></ul>
Spring 2017	<p><i>Student Teacher, Harborside Academy, Kenosha, WI</i></p> <ul style="list-style-type: none"><li>• Taught 10<sup>th</sup> grade Chemistry classes for half a semester</li></ul>
Jan 2016 – Aug 2016	<p><i>Undergraduate Teaching Lab Researcher, Carthage College, Kenosha, WI</i></p> <ul style="list-style-type: none"><li>• Adapted and developed nanoparticle-based experiments into labs to help demonstrate various chemistry topics and reactions within time restrictions for organic and general chemistry classes'</li></ul>
Sep 2015 – May 2016	<p><i>Chemistry Tutor, Carthage College, Kenosha, WI</i></p> <ul style="list-style-type: none"><li>• Tutored students in General Chemistry and Organic Chemistry</li></ul>

## Selected Teaching Awards and Honors

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July 2021	<p><b>CIRTL Scholar certification</b>, University of Iowa</p> <p>Awarded for adding to community knowledge about teaching and learning by presenting findings from a <i>Teaching as Research</i> (TAR) project after obtaining a Center for the Integration of Research, Teaching and Learning (CIRTL) Practitioner's certification</p>
May 2019	<p><b>Outstanding Teaching Assistant Award</b>, University of Iowa</p> <p>Awarded by the Council on Teaching for excellence in teaching</p>
Spring 2016	<p><b>Judith Schaumberg Scholarship</b>, Carthage College</p> <p>Awarded by the Department of Education for excellence and demonstrated passion for teaching</p>

## Other Professional Experience

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July 2021	Telluride School on Theoretical Chemistry, <b>Telluride, CO</b>
Aug 2020 – May 2021	Teaching and Research (TAR) project conducted on a Quantum Chemistry class, <b>University of Iowa, Iowa City, IA</b>
October 2020	NERSC Parallelware Training Series: Motif-guided Parallelization of ZPIC with OpenMP and OpenACC, <b>Online training workshop</b>
July 2019	MolSSI Stochastic Approaches to Electronic Structure Calculations Workshop, <b>University of Pittsburgh, Pittsburgh, PA</b>
July 2017	POGIL 2018 South Central Regional Workshop, <b>University of Texas at Dallas, Richardson, TX</b>

## Publications

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- 6.** Weiler, L; **Mihm, T.**; and Shepherd, J. J. “Machine learning for a finite size correction in periodic coupled cluster theory calculations” in preparation
- 5.** **Mihm, T**; Weiler, L; and Shepherd, J. J. “Correcting for errors in the correlation energy using the exchange structure factor” in progress
- 4.** **Mihm, T**; Schäfer, T.; Ramadugu, S. K.; Weiler, L.; Grüneis, A.; and Shepherd, J. J. “A shortcut to the thermodynamic limit for quantum many-body calculations of metals”. *Nat Comput Sci* **1**, 801–808 (2021). <https://doi.org/10.1038/s43588-021-00165-1>
- 3.** **Mihm, T**; Yang, B; Shepherd, J. J. “Power laws used to extrapolate the coupled cluster correlation energy to the thermodynamic limit”, *J. Chem. Theory Comput.* **17**, 5, 2752–2758 (2021); <https://doi.org/10.1021/acs.jctc.0c01171>
- 2.** **Mihm, T.**; Van Benschoten, W. Z.; Shepherd, J. J. “Accelerating convergence to the thermodynamic limit with twist angle selection applied to methods beyond many-body perturbation theory”. *J. Chem. Phys.* **154**, 024113 (2021); (Invited) <https://doi.org/10.1063/5.0033408>
- 1.** **Mihm, T.**; McIsaac, A. R.; Shepherd, J. J. “An optimized twist angle to find the thermodynamic limit derived from the uniform electron gas”. *J. Chem. Phys.* **150**, 191101 (2019); <https://doi.org/10.1063/1.5091445>

## Oral Presentations

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- 5.** **Mihm, T.**; Schäfer, T.; Weiler, L.; Ramadugu, S. K.; Grüneis, A.; Shepherd, J. J. *Applying coupled cluster theory to real metals using structure factor twist averaging* presented at the American Chemical Society Spring 2021 Meeting, online
- 4.** **Mihm, T.**; Van Benschoten, W. Z.; Ramadugu, S. K.; Grüneis, A.; Shepherd, J. J. *Applying connectivity twist averaging to quantum Monte Carlo and real solids* presented at the American Physical Society March Meeting 2021, online
- 3.** **Mihm, T**; Yang, B; Shepherd, J. J. *What can the transition structure factor tell us about finite size effects in metals?*, presented as a recorded lightning talk at the Virtual Conference on Theoretical Chemistry 2020, Hosted by Stanford University, Stanford, CA, online

**2. Mihm, T;** Shepherd, J J. *Stochastic Methods in Electronic Structure Theory, A Simpler Twist Averaging for use in Uniform Electron Gas and Real System Calculations*, presented at the Telluride Science Research Center Stochastic Methods in Electronic Structure Theory 2019 workshop, Telluride, CO

**1. Mihm, T;** McIsaac, A. R.; Shepherd, J. J. *A simpler twist averaging for the uniform electron gas designed for finite basis set calculations such as coupled cluster and full configuration interaction quantum Monte Carlo*, presented at the American Physical Society March Meeting 2019, Boston, MA

## Posters

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**8. Mihm, T.;** Yang, B.; Weiler, L.; Schäfer, T.; Ramadugu, S. K.; Grüneis, A.; Shepherd, J. J. Virtual Poster: *Improving periodic coupled cluster theory using the transition structure factor* presented at the American Chemical Society Fall 2021 Meeting, Atlanta, GA

**7. Mihm, T;** Weiler, L.; Van Benschoten, W. Z.; Ramadugu, S. K.; Schäfer, T.; Grüneis, A.; Shepherd, J. J. Virtual Poster: *Twist angle selection in full configuration interaction quantum Monte Carlo and coupled cluster theory for solids*, presented at the Telluride Science Research Center Stochastic Methods in Electronic Structure Theory 2021 virtual workshop, Hosted by Telluride, CO

**6. Mihm, T.;** Petras, H.; Scharlott, L; Weiler, L; Smith, A; Rodriguez, J-M; Al Lawati, R.; Becker, N; Shepherd, J. J. Virtual Poster: *A Scholarship of Teaching and Learning study of an upper-division Physical Chemistry classroom at the University of Iowa*, presented at National Convention for Advanced POGIL Practitioners meeting 2021

**5. Mihm, T.,** Yang, B., Shepherd, J. J. Virtual Poster: *Evaluating the convergence rate of the finite size effects in the thermodynamic limit of connectivity-twist-averaged coupled cluster calculations in the uniform electron gas*. presented at Virtual Electronic Structure Workshop 2020, University of California - Merced, Merced, CA

**4. Mihm, T;** Yang, B; Shepherd, J J. Poster: *What can the transition structure factor tell us about finite size effects in metals?*, presented alongside lightning talk at the Virtual Conference on Theoretical Chemistry 2020, Hosted by Stanford University, Stanford, CA. online

**3. Mihm, T.;** Petras, H.; Shepherd, J. J. Poster: *Reflecting on using visual simulations of quantum mechanics to supplement POGIL classroom activities in upper-division Physical Chemistry classrooms at the University of Iowa*, presented at National Convention for Advanced POGIL Practitioners meeting 2019, Washington University, St. Louis, MO

**2. Mihm, T;** Ramadugu, S. K.; McIsaac, A. R.; Grüneis, A.; Shepherd, J. J Poster: *Developing the coupled cluster method in the VASP software package*, presented at American-Mexican Symposium on Supramolecular Materials Design 2019, University of Iowa, Iowa City, IA

**1. Mihm, T;** Ramadugu, S. K.; McIsaac, A. R.; Grüneis, A.; Shepherd, J. J Poster: *Developing a twist-averaged coupled cluster method in the VASP software package*, presented at American Chemical Society UI Student Chapter Symposium Design 2019, University of Iowa, Iowa City, IA

## Skills

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- Proficient in Python, FORTRAN and Bash programming languages
- Proficient in running Vienna Ab initio Simulation Package (VASP)
- Familiar with Highly Accurate N-Determinant quantum Monte Carlo software (HANDE)

## Professional Affiliations

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2018 - present	American Physical Society (APS)
2017 - present	American Chemical Society (ACS)

## Leadership

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2019 - 2020	Mentor for Women in Science and Engineering (WISE) mentor program, <b>University of Iowa</b> <ul style="list-style-type: none"><li>- Mentored undergraduate female STEM students through their first year of college</li><li>- Attended mentorship training for mentoring women in STEM fields</li></ul>
2015 - 2016	Outreach coordinator for Chemistry Club, <b>Carthage College</b> <ul style="list-style-type: none"><li>- Coordinated and ran science demonstrations and events with local libraries and schools to help build kid's interests in STEM</li><li>- Coordinated and ran science demonstrations on campus</li></ul>