

# Craig Waitt

Ph.D. Candidate

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## Education

Jan 2018 – Dec 2022 (Expected)	<b>University of Notre Dame, Notre Dame</b> <i>Ph.D. in Chemistry</i>
Sep 2015 – May 2017	<b>Montclair State University, Montclair</b> <i>MSc in Chemistry</i>
Sep 2010 – May 2015	<b>Montclair State University, Montclair</b> <i>BSc in Chemistry</i> <i>ACS certified</i>

## Research Experience

Jan 2018 – May 2022 (Expected)	<b>Graduate Research Assistant - University of Notre Dame</b> <i>Computational Catalytic Chemist</i> <ul style="list-style-type: none"><li>• Design computational models to describe/explain chemical phenomena</li><li>• Develop python modules to streamline research objectives<ul style="list-style-type: none"><li>– Created several python modules to increase productivity and efficiency</li><li>– Modules have been made freely available on GitHub</li></ul></li><li>• Mentor junior/upcoming graduate and undergraduate students</li><li>• Facilitate collaborations between, experimental, industrial, and computational, research groups to advance research objective<ul style="list-style-type: none"><li>– Collaborations include: Groups within the University of Notre Dame, Purdue University, and BASF</li></ul></li></ul> <p><i>Projects</i></p> <ul style="list-style-type: none"><li>• Benchmarking popular free energy and entropy models on surfaces against a new, novel approach</li><li>• Designing python modules to solve the Schrödinger equation for students, teachers, and researchers</li><li>• Understanding the relationship between templating molecules, zeolites, and the resulting distribution of silica and alumina</li><li>• Elucidating the dealumination mechanism in zeolites</li><li>• Modeling the spectra <math>\text{NH}_x</math> species under plasma synthesis conditions</li></ul>
Jan 2014 – July 2017	<b>Graduate Research Assistant - Montclair State University</b> <i>Computational Chemist</i> <ul style="list-style-type: none"><li>• Design computational models to describe/explain chemical phenomena</li><li>• Benchmark tools and write protocols for future students to use to streamline research objectives</li></ul> <p><i>Projects</i></p> <ul style="list-style-type: none"><li>• A Computational Study of C-CN Bond Activation through Nickel Catalysis using the Random Phase Approximation</li></ul>

## Teaching Experience

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Sep 2021 – May 2022	<b>Navari Family Center for Digital Scholarship (NFCDS) Fellow - University of Notre Dame</b> <ul style="list-style-type: none"><li>• Design and facilitate workshops open to students, faculty, and staff at the University of Notre Dame<ul style="list-style-type: none"><li>– "An Introduction of <math>\LaTeX</math> for the Curious"</li><li>– "Writing your Dissertation or Thesis in <math>\LaTeX</math>"</li></ul></li></ul>
Sep 2017 – July 2019	<b>Graduate Teaching Assistant - University of Notre Dame</b> <ul style="list-style-type: none"><li>• Guided students through problem worksheets and hosted personal office hours<ul style="list-style-type: none"><li>– General Chemistry</li><li>– Organic Chemistry</li><li>– Physical Chemistry</li><li>– Science and Engineering Scholar Principles of Chemistry</li></ul></li><li>• Implemented new grading software to improve and streamline student-teacher communication for assignments and exams</li></ul>
Sep 2015 – May 2019	<b>Graduate Teaching Assistant - Montclair State University</b> <ul style="list-style-type: none"><li>• Guided students through problem worksheets and hosted personal office hours<ul style="list-style-type: none"><li>– Principles of Chemistry Laboratory (non-science majors)</li></ul></li><li>• Prepare chemicals and materials for laboratory use</li><li>• Grade and assist in writing new laboratory reports</li></ul>

## Awards, Grants, and Honors

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Sep 2021	The Navari Family Center for Digital Scholarship Pedagogy Fellowship
May 2019	Rudy Bottei Graduate Teaching Award
May 2016	Margaret and Herman Graduate Summer Research Fellowship
Sep 2010	Margaret and Herman Freshman Scholarship

## Publications

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2022	1. Yan, C., <b>Waitt, C.</b> , Akintola, I., Lee, G., Easa, J., Clarke, R., Geng, F., Poirier, D., Otor, H. O., Rivera-Castro, G., Go, D. B., O'Brien, C. P., Hicks, J. C., Schneider, W. F. & Ma, H. Recent Advances in Plasma Catalysis. <i>Industrial &amp; Engineering Chemistry Research</i> <b>61</b> , 7675–7678. eprint: <a href="https://doi.org/10.1021/acs.iecr.2c01594">https://doi.org/10.1021/acs.iecr.2c01594</a> (2022).
2021	2. Barboun, P. M., Daemen, L. L., <b>Waitt, C.</b> , Wu, Z., Schneider, W. F. & Hicks, J. C. Inelastic Neutron Scattering Observation of Plasma-Promoted Nitrogen Reduction Intermediates on Ni/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub> . <i>ACS Energy Letters</i> <b>6</b> , 2048–2053 (2021). 3. <b>Waitt, C.</b> , Miles, R. A. & Schneider, W. F. Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes. <i>J. Phys. Chem. C</i> <b>125</b> , 20331–20342 (2021).
2017	4. Tummalapalli, S. R., Bhat, R., <b>Waitt, C.</b> , Eshuis, H. & Rotella, D. P. Synthesis and computational analysis of conformationally restricted [3.2. 2]-and [3.2. 1]-3-azabicyclic diamines. <i>Tetrahedron Letters</i> <b>58</b> , 4087–4089 (2017).
2016	5. <b>Waitt, C.</b> , Ferrara, N. M. & Eshuis, H. Thermochemistry and geometries for transition-metal chemistry from the random phase approximation. <i>Journal of Chemical Theory and Computation</i> <b>12</b> , 5350–5360 (2016).

## **Presentations**

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August 2022	<b>ACS Fall 2022: American Chemical Society</b> <ul style="list-style-type: none"><li>• Exploring the Relationship Between Organic Structure Directing Agents and Al Distribution in CHA</li><li>• Presentation Type: Oral</li></ul>
May 2022	<b>NAM 27: 2022 North American Catalysis Society</b> <ul style="list-style-type: none"><li>• Exploring the Relationship Between Organic Structure Directing Agents and Al Distribution in CHA</li><li>• Presentation Type: Poster</li></ul>
April 2021	<b>ACS Spring 2021: American Chemical Society</b> <ul style="list-style-type: none"><li>• Moving beyond the Harmonic Oscillator and Hindered Translator Models to Compute Free Energies and Entropies of Surface-bound Species</li><li>• Presentation Type: Oral</li></ul>
June 2019	<b>NAM 26: 2019 North American Catalysis Society Meeting</b> <ul style="list-style-type: none"><li>• Benchmarking Adsorbate Free Energies and Their Reliability to Determine Equilibrium Constants and Microkinetic Rates</li><li>• Presentation Type: Poster</li></ul>

## **References**

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**Available Upon Request**