

Craig Waitt, Ph.D.

Postdoctoral Fellow

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Education

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

Research Experience

Jan 2023 – Current	Postdoctoral Fellow - University of Notre Dame <i>Computational Catalytic Chemist</i> <ul style="list-style-type: none">• Develop models to understand catalytic problems using computational methods, including density functional theory (DFT) and molecular dynamics simulations to design and optimize catalyst performance to aid in environmental pollutant abatement• Collaborate with experimentalists to design and interpret experiments related to catalysis• Publish and review papers in top-tier chemistry journals• Mentor junior/upcoming graduate and undergraduate students• Present research at national conferences <i>Projects</i> <ul style="list-style-type: none">• Model CHA-zeolites under hydrothermal conditions to understand how dealumination can be tuned for desired catalytic properties
Jan 2018 – Dec 2022	Graduate Research Assistant - University of Notre Dame <i>Computational Catalytic Chemist</i> <ul style="list-style-type: none">• Develop python modules to streamline research objectives<ul style="list-style-type: none">– Created several python modules to increase productivity and efficiency– Modules have been made freely available on GitHub• Mentor junior/upcoming graduate and undergraduate students• Facilitate collaborations between, experimental, industrial, and computational, research groups to advance research objective<ul style="list-style-type: none">– Collaborations include: Groups within the University of Notre Dame, Purdue University, and BASF <i>Projects</i> <ul style="list-style-type: none">• Benchmarking popular free energy and entropy models on surfaces against a new, novel approach• Designing python modules to solve the Schrödinger equation for students, teachers, and researchers• Understanding the relationship between templating molecules, zeolites, and the resulting distribution of silica and alumina• Elucidating the dealumination mechanism in zeolites• Modeling the spectra NH_x species under plasma synthesis conditions

Jan 2014 – July 2017	Graduate Research Assistant - Montclair State University <i>Computational Chemist</i> <ul style="list-style-type: none"> • Design computational models to describe/explain chemical phenomena • Benchmark tools and write protocols for future students to use to streamline research objectives <i>Projects</i> <ul style="list-style-type: none"> • A Computational Study of C-CN Bond Activation through Nickel Catalysis using the Random Phase Approximation
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Teaching Experience

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

Awards, Grants, and Honors

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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| 2023 | 1. Waitt, C. , Gao, X., Gounder, R., Debellis, A., Prasad, S., Moini, A. & Schneider, W. F. Analysis and Augmentation of Guest–Host Interaction Energy Models as CHA and AEI Zeolite Crystallization Phase Predictors. <i>J. Phys. Chem. C</i> 127 , 22740–22741 (2023). |
| 2022 | 2. Yan, C., Waitt, C. , 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 & Engineering Chemistry Research</i> 61 , 7675–7678 (2022). |
| 2021 | 3. Barboun, P. M., Daemen, L. L., Waitt, C. , Wu, Z., Schneider, W. F. & Hicks, J. C. Inelastic Neutron Scattering Observation of Plasma-Promoted Nitrogen Reduction Intermediates on Ni/ γ -Al ₂ O ₃ . <i>ACS Energy Letters</i> 6 , 2048–2053 (2021). |
| | 4. Waitt, C. , Miles, R. A. & Schneider, W. F. Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes. <i>J. Phys. Chem. C</i> 125 , 20331–20342 (2021). |
| 2017 | 5. Tummalapalli, S. R., Bhat, R., Waitt, C. , 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> 58 , 4087–4089 (2017). |
| 2016 | 6. Waitt, C. , 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> 12 , 5350–5360 (2016). |

Presentations

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| March 2023 | ACS Spring 2023: American Chemical Society <ul style="list-style-type: none">• Analysis and Augmentation of Guest-Host Interaction Energy Models as CHA and AEI Zeolite Crystallization Phase Predictors• Presentation Type: Oral |
| August 2022 | ACS Fall 2022: American Chemical Society <ul style="list-style-type: none">• Exploring the Relationship Between Organic Structure Directing Agents and Al Distribution in CHA• Presentation Type: Oral |
| May 2022 | NAM 27: 2022 North American Catalysis Society <ul style="list-style-type: none">• Exploring the Relationship Between Organic Structure Directing Agents and Al Distribution in CHA• Presentation Type: Poster |
| April 2021 | ACS Spring 2021: American Chemical Society <ul style="list-style-type: none">• Moving beyond the Harmonic Oscillator and Hindered Translator Models to Compute Free Energies and Entropies of Surface-bound Species• Presentation Type: Oral |
| June 2019 | NAM 26: 2019 North American Catalysis Society Meeting <ul style="list-style-type: none">• Benchmarking Adsorbate Free Energies and Their Reliability to Determine Equilibrium Constants and Microkinetic Rates• Presentation Type: Poster |

References

Available Upon Request