Craig Waitt, Ph.D.

Postdoctoral Fellow

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Education

Jan 2018 – Dec 2022 | **University of Notre Dame, Notre Dame**
Ph.D. in Chemistry

Sep 2015 – May 2017 | **Montclair State University, Montclair**
MSc in Chemistry

Sep 2010 – May 2015 | **Montclair State University, Montclair**
BSc in Chemistry
ACS certified

Research Experience

Jan 2023 – Current | **Postdoctoral Fellow - University of Notre Dame**
Computational Catalytic Chemist

- Develop models to understand catalytic problems using computational methods, including density functional theory (DFT) and molecular dynamics simulations
- 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

Projects

- 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**
Computational Catalytic Chemist

- Develop python modules to streamline research objectives
  - 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
  - Collaborations include: Groups within the University of Notre Dame, Purdue University, and BASF

Projects

- 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

Computational Chemist

- Design computational models to describe/explain chemical phenomena
- Benchmark tools and write protocols for future students to use to streamline research objectives

Projects

- A Computational Study of C-CN Bond Activation through Nickel Catalysis using the Random Phase Approximation

Teaching Experience

Sep 2021 – May 2022

Navari Family Center for Digital Scholarship (NFCDS) Fellow - University of Notre Dame

- Design and facilitate workshops open to students, faculty, and staff at the University of Notre Dame
  - "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

- Guided students through problem worksheets and hosted personal office hours
  - 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

- Guided students through problem worksheets and hosted personal office hours
  - 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

2022
1. 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. *Industrial & Engineering Chemistry Research* **61,** 7675–7678. eprint: `https://doi.org/10.1021/acs.iecr.2c01594` (2022).

2021
2. 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_2O_3. *ACS Energy Letters* **6,** 2048–2053 (2021).
3. **Waitt, C.**, Miles, R. A. & Schneider, W. F. Adsorbate Free Energies from DFT-Derived Translational Energy Landscapes. *J. Phys. Chem. C* **125,** 20331–20342 (2021).

2017
4. 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. *Tetrahedron Letters* **58,** 4087–4089 (2017).

2016
5. **Waitt, C.**, Ferrara, N. M. & Eshuis, H. Thermochemistry and geometries for transition-metal chemistry from the random phase approximation. *Journal of Chemical Theory and Computation* **12,** 5350–5360 (2016).

Presentations

March 2023 | **ACS Spring 2023: American Chemical Society**
- 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**
- 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**
- Exploring the Relationship Between Organic Structure Directing Agents and Al Distribution in CHA
- Presentation Type: Poster

April 2021 | **ACS Spring 2021: American Chemical Society**
- 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**
- Benchmarking Adsorbate Free Energies and Their Reliability to Determine Equilibrium Constants and Microkinetic Rates
- Presentation Type: Poster

References

Available Upon Request