Joseph P. Fernandez

University of Cincinnati | fernajp@uc.edu | josephpfernandez.com | 513-600-7978

Current Employment

Post Doctoral Fellow, University of Cincinnati 2022 – Present

- Research Fellow in the Procter & Gamble Digital Accelerator at University of Cincinnati, College of Engineering and Applied Science
- Innovating in computational chemistry and environmental engineering through the development of simulations to rapidly predict the experimental outcomes of biodegradable polymers toward advancing efforts in creating sustainable consumer materials.

Education

The Ohio State University 2017 – 2023

- **Ph.D.**, Organic Chemistry Division of the Chemistry Graduate Program
- Areas of Expertise: computational chemistry, molecular modelling, drug discovery, enzyme-ligand interaction analysis, organic mechanism elucidation, statistical thermodynamics
- Technical Skills: applications in quantum mechanics (*Gaussian*) and molecular dynamics (*Schrödinger, AMBER, AutoDock*), high throughput screening data analysis (*python, matplotlib, Jupyter, rdkit*), and HPC (*Unix, bash*)

The Ohio State University 2007 – 2011

- **B.A.**, Chemistry *with Honors in the Arts and Sciences*
- **B.A.**, Philosophy *with Honors in the Arts and Sciences*

Research Experience

Post Doc Fellow, P&G Digital Accelerator @ UC 2022 – Present

- Designed docking and molecular dynamics (*Schrödinger*) simulations of microbial enzymes and polymeric substrates to understand and predict biodegradation pathways in wastewater treatment facilities.
- Created polymer biodegradation model (*python, Jupyter*) to accurately and rapidly reproduce ($R^2 > 0.8$) the outcomes of experimental biodegradation data (*OECD 301B*) on over 100 natural and synthetically functionalized polymers.
- Expanded polymer biodegradation model capability through the implementation of Markov chain algorithm to investigate the effects of varying polymer composition on metabolite distribution and biodegradation.
- Developed code and graphical user interface for accessible usage of polymer biodegradation model as an internal web application (*Streamlit*) to dramatically improve design time by reducing reliance on costly and drawn-out experiments.
- Authored multiple articles describing the proprietary IP of the novel polymer biodegradation model in the P&G internal learning report system.

Graduate Research Associate, The Ohio State University 2017 – 2022

Dissertation Advisor: Dr. Christopher Hadad

- Applications of computational chemistry simulations to predict physical properties of novel organic molecules and complex biochemical systems.
- Design and analysis of novel therapeutics for organophosphorus poisoning of acetylcholinesterase
- Develop innovative and useful high throughput binding energy analyses and graphical representations.
- Organic reaction mechanism elucidation through free energy calculations and transition state theory

Student Research Associate, The Ohio State Medical Center, Leukemia Tissue Bank 2008 – 2011

PI: Dr. Michael Caligiuri

- Central collection, processing, storage, and characterization of tissue samples and derivatives (plasma, serum, DNA, RNA, protein) from patients with any hematologic malignancies

Publications

Sahraeian, T.; Kulyk, D. S.; **Fernandez, J. P**.; Hadad, C. M.; Badu-Tawiah, A. K. Capturing Fleeting Intermediates in a Claisen Rearrangement Using Nonequilibrium Droplet Imbibition Reaction Conditions. Anal. Chem. 2022, 94 (43), 15093–15099. https://doi.org/10.1021/acs.analchem.2c03268.

Scott, S.; **Fernandez, J. P**.; Hadad, C. M.; MacKay, A. "Molecular Docking as a Tool to Examine Organic Cation Sorption to Organic Matter" Environ. Sci. Technol. 2022, 56(2), 951 – 961, doi:10.1021/acs.est.1c06147

Wolfson, E. R.; Schkeryantz, L.; Moscarello, E. M.; **Fernandez, J. P**.; Paszek, J.; Wu, Y.; Hadad, C. M.; McGrier, P. L. "Alkynyl-Based Covalent Organic Frameworks as High-Performance Anode Materials for Potassium-Ion Batteries" ACS Appl. Mater. Interfaces 2021, 13(35), 41628 – 41636, doi: 10.1021/acsami.1c10870

Gunther, M. J.; Pavlović, R. Z.; **Fernandez, J. P**.; Zhiquan, L.; Gallucci, J.; Hadad, C. M.; Badjić, J. D. "Stereo- and Regioselective Synthesis of Molecular Baskets" J. Org. Chem. 2019, 84(7), 4392 – 4401, doi:10.1021/acs.joc.9b00330 \

Parkin, S. R.; Coldren, W. H.; **Fernandez, J. P**.; Hadad, C. M.; Behrman, E. J. "Polymorphism, Crystal Packing, Twinning, and Molecular Conformations in 5'-Halo-5'-deoxyguanosines and a Hydrate of the Pseudo-halide Analogue, 5'-Azido-5'-deoxyguanosine" Crystal Growth & Design. 2018, 18(11), 6995 – 7005, doi:10.1021/acs.cgd.8b01162

Presentations

Fernandez, J.P.; Franjesevic, A.J.; Coldren, W.H.; Nosseir, O.; Zhuang, Q.; Hadad, C.M. Molecular Conformations in the Active Site of Organophosphorus-Aged Acetylcholinesterase: Insights into the Rational Development of Nerve Agent Countermeasures. *Selected Oral Presentation* at the Gordon Research Conference: Detection, Countermeasures, and Prevention of Chemical and Biological Threats; Ventura, CA; March 2019

Awards & Honors

John S. Swenton Award for Outstanding Teaching 2021
Awarded to the top graduate teaching associate for excellence in classroom instruction

Grants & Fellowships

GAANN Fellowship 2019
Graduate Enrichment Fellowship 2017 – 2018

Teaching Experience

The Ohio State University

- Develop new teaching material and laboratory experiments, mentor undergraduate teaching assistants.
- Instruct (virtual and in person) and grade regular coursework:
- General Chemistry I&II, Organic Chemistry I&II, Computational Chemistry, Spectroscopy of Organic Compounds

Graduate Teaching Associate 2017, 2018, 2021
Staff Teaching Associate 2011– 2013, 2016 – 2017

Service

Ohio-5 SURE Mentor 2021
Industry Day Host 2018
Prospective Student Host 2017, 2018

Professional Affiliations

American Chemical Society

Additional Technical Skills

Microsoft Office, LLM, ChatGPT, ML/AI, Web Development, Graphics Processing