

ZACKARY FALLS

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EDUCATION

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| 2012 – PRESENT | Doctor of Philosophy (Ph.D.) in COMPUTATIONAL CHEMISTRY
University at Buffalo, State University of New York , Buffalo, New York
Thesis: “Elucidating Chemical Structures via DFT Investigations”
— Advisor: Prof. Eva Zurek |
| 2008 – 2012 | Bachelor of Science (B.S.) in CHEMISTRY – ACS Accredited
Canisius College , Buffalo, New York |

RESEARCH EXPERIENCE

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| Current
2012 – PRESENT | Graduate Researcher at University at Buffalo, State University of New York
— Advisor: Eva Zurek

Primary research topic involves the molecular modeling of homogeneous and heterogeneous polyolefin polymerization catalyzed by single-site metallocene complexes. Metallocenes need to be activated by a co-catalyst such as methylaluminoxane (MAO) in order for polymerization to occur. The structure(s) of MAO have remained a mystery despite several experimental and theoretical studies. Computational methods are employed to explore the dynamic equilibria of various plausible MAO oligomers and structural entities for this elusive, yet significant, co-catalyst. We are continuing to study the interaction of MAO oligomers with $MgCl_2$ support. Our secondary project involves further development of, XTALOPT, an open source evolutionary algorithm for crystal structure prediction. |
| 2011 – 2012 | Undergraduate Researcher at Canisius College
— Advisor: Jeremy Steinbacher

Research in the field of bio-organic material synthesis, specifically mesoporous silica nanoparticles. Qualitative and quantitative analyses were employed for these products using thermogravimetric analysis, thin-layer chromatography, nuclear magnetic resonance, and other methods. Employed techniques to synthesize functionalized polyhedral oligomeric silsesquioxanes. |
| SUMMER 2011 | Undergraduate Researcher at University at Buffalo, State University of New York
<i>Research Education for Undergraduates</i>
— Advisor: Eva Zurek

Ten week program to allow for the experience of graduate level research as an undergraduate. Research focused on testing a newly written random docking algorithm to screen a library of possible monomers used for molecularly imprinted polymers/xerogels. |

PUBLICATIONS

- **Falls, Z.**; Lonie, D. L.; Avery, P.; Shamp, A.; Zurek, E. “XTALOPT version r9: An opensource evolutionary algorithm for crystal structure prediction” *Comp. Phys. Comm.* 2015, *In Press*. doi: 10.1016/j.cpc.2015.09.018
- Shamp, A.; Terpstra, T.; Bi, T.; **Falls, Z.**; Avery, P.; Zurek, E. “Decomposition Products of Phosphine Under Pressure: PH_2 Stable and Superconducting?”, 2015, *Preprint*. arXiv:1509.05455.
- **Falls, Z.**; Tyminska, N.; Zurek, E. “The Dynamic Equilibrium Between $(AlOMe)_n$ Cages and $(AlOMe)_n \cdot (AlMe_3)_m$ Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation”, *Macromolecules*. 2014, 47 (24), 85568569. doi: 10.1021/ma501892v
- Wach, A.; Chen, J.; **Falls, Z.**; Lonie, D.; Mojica, E.; Aga, D.; Autschbach, J.; Zurek, E. “Determination of the Structures of Molecularly Imprinted Polymers and Xerogels Using an Automated Stochastic Approach”, *Anal. Chem.* 2013, 85 (18), 8577-8584. doi: 10.1021/ac402004z

TEACHING EXPERIENCE

Current 2012 – PRESENT	Teaching Assistant at University at Buffalo, State University of New York General Chemistry
SPRING 2012	Teaching Assistant at Canisius College General Chemistry
FALL 2011	Teaching Assistant at Canisius College Analytical Chemistry

AWARDS RECEIVED

2012 – 2015	Gordon Harris Fellowship Award University at Buffalo, State University of New York
2013	Graduate Student Employees Union Professional Development Award University at Buffalo, State University of New York
2012 – 2013	Marjorie Winkler Fellowship Award University at Buffalo, State University of New York
2012	Merck Index Award Canisius College
2012	REU Chemistry Leadership Award National Science Foundation

CONFERENCES ATTENDED

JULY 2014	Gordon Research Conference – Atomic and Molecular Interactions <i>“Exploring the Dynamic Equilibrium between MAO (methylaluminoxane) Oligomers via First Principles Calculations”</i> Poster
MAY 2014	Graduate Student Symposium – University at Buffalo, State University of New York <i>“Exploring the Dynamic Equilibrium between MAO (methylaluminoxane) Oligomers via First Principles Calculations”</i> Presentation
MAY 2013	Canadian Chemistry Conference – Canadian Society for Chemistry <i>“Computations of the Equilibria between various MAO, (AlOMe)_n, Oligomers and their EFG Tensors”</i> Poster
MAY 2013	Graduate Student Symposium – University at Buffalo, State University of New York <i>“Analysis of Electric Field Gradient Tensors at the Quadrupolar Aluminum Nuclei for Oligomers of Methylaluminoxane”</i> Poster
OCTOBER 2012	American Chemical Society – Northeast Regional Meeting <i>“Interactions in Cp₂ZrMe₂-catalyzed, MAO (methylaluminoxane) Catalyzed Heterogeneous Polymerization: A Computational Approach”</i> Poster
MARCH 2012	American Chemical Society – National Meeting <i>“Computational Analysis of Imprinting Polymers and Xerogels using a Random Docking Program”</i> Poster