ZACKARY FALLS

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EDUCATION

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

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**
Research Education for Undergraduates
— 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** *"Exploring the Dynamic Equilibrium between MAO (methylaluminoxane) Oligomers via First Principles Calculations"* Poster
MAY 2014	Graduate Student Symposium – **University at Buffalo, State University of New York** *"Exploring the Dynamic Equilibrium between MAO (methylaluminoxane) Oligomers via First Principles Calculations"* Presentation
MAY 2013	Canadian Chemistry Conference – **Canadian Society for Chemistry** *"Computations of the Equilibria between various MAO, $(AlOMe)_n$, Oligomers and their EFG Tensors"* Poster
MAY 2013	Graduate Student Symposium – **University at Buffalo, State University of New York** *"Analysis of Electric Field Gradient Tensors at the Quadrupolar Aluminum Nuclei for Oligomers of Methylaluminoxane"* Poster
OCTOBER 2012	American Chemical Society – **Northeast Regional Meeting** *"Interactions in Cp_2ZrMe_2–catalyzed, MAO (methylaluminoxane) Catalyzed Heterogeneous Polymerization: A Computational Approach"* Poster
MARCH 2012	American Chemical Society – **National Meeting** *"Computational Analysis of Imprinting Polymers and Xerogels using a Random Docking Program"* Poster