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 in CHEMISTRY – ACS Accredited
Canisius College, Buffalo, New York
Cum Laude

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. Synthesis of 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.; Tyminska, N.; Zurek, E. The Dynamic Equilibrium Between (AlOMe)n Cages and (AlOMe)n(AlMe3)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

JUL 2010-OCT 2011	Summer Intern at INTECH INC, Chicago Received pre-placed offer from the Exotics Trading Desk as a result of very positive review. Rated "*truly distinctive*" for Analytical Skills and Teamwork.

AWARDS RECEIVED

SEPT. 2012	Faculty of Science Masters Scholarship ($30,000)

CONFERENCES ATTENDED

COMPUTER SKILLS

Basic Knowledge:	PHP, mySQL, HTML, Access, LINUX, ubuntu
Intermediate Knowledge:	VBA, Excel, Word, PowerPoint