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1 Zackary Falls

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2 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

3 Research Experience

<i>Current</i> 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 <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.

4 Publications

- Falls, Z.; Tyminska, N.; Zurek, E. The Dynamic Equilibrium Between $(AlOMe)_n$ Cages and $(AlOMe)_n(AlMe_3)_m$ 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

7 Conferences Attended

8 Computer Skills

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