

Brett A. Smith

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EDUCATION

The University of Tennessee, Knoxville	Ph.D., Chemistry Supervised by Dr. Konstantinos Vogiatzis	August 2018 – December 2022
The University of South Carolina Aiken	Bachelor of Science, Chemistry Supervised by Dr. Gerard T. Rowe	August 2014 – May 2018

PEER REVIEWED PUBLICATIONS

- (1) Schneider, J. D.; Smith, B. A.; Williams, G. A.; Powell, D. R.; Perez, F.; Rowe, G. T.; Yang, L. Synthesis and Characterization of Cu(II) and Mixed-Valence Cu(I)Cu(II) Clusters Supported by Pyridylamide Ligands. *Inorg. Chem.*, **2020**, 59, 5433-5446
- (2) Liu, S.; Smith, B. A.; Kirkland, J. K.; Vogiatzis, K. D.; Girolami, G. S. Nature of the Short Rh-Li Contact between Lithium and the Rhodium ω -Alkenyl Complex [Rh(CH₂CMe₂CH₂CH=CH₂)₂]-. *Inorg. Chem.*, **2021**, 60 (12), 8790–8801.
- (3) Smith, B. A.; Vogiatzis, K. D. σ -Donation and π -Backdonation Effects in Dative Bonds of Main-Group Elements. *J. Phys. Chem. A.*, **2021**, 125 (36), 7956–7966.
- (4) Jones*, G. J.; Smith*, B. A.; Kirkland, J.K.; Townsend, J. A.; Vogiatzis, K.D. Data-Driven Ligand Field Engineering of Fe(IV)-oxo Sites for C-H Activation. *Inorg. Chem. Front.*, **2022**, Accepted Manuscript

MANUSCRIPTS IN PREPARATION

- (1) Wilson, B.J.; Smith, B. A.; Vogiatzis, K. D.; Brantley, J. Selectivity and Tacticity of Asymmetrically Metal Carbonyl Functionalized Norbornene in Ring Opening Polymerization Metathesis Polymerization
Manuscript in Preparation
- (2) Smith, B.A.; Jenkins, D.M., Vogiatzis, K.D. Computational Examination of Iron Tetra N-Heterocyclic Carbene Reactivity for Catalytic Aziridination. *Manuscript In Preparation*
- (3) Russell, J.J.; Smith, B.A.; Vogiatzis, K.D.; Jenkins, D.M. Reactivity and Mechanism of Imide Insertion in Chiral Iron Tetracarbene Fused Macrocyclic. *Manuscript in Preparation*

PRESENTATIONS

- High-throughput screening of metal tetracarbene complexes for enantioselective aziridination catalysis”, National ACS Meeting. March, 2022. Oral Presentation
- “In Silico Design and High-Throughput Screening of 2D Monolayer and Stacked Bilayer Van der Waals Heterostructure Materials”, Original Research Proposal. November, 2021. Oral Presentation.
- “Highly Accurate Benchmarking and Characterization of Donor-Acceptor Interactions in Molecular Systems Containing Dative Bonds”, National ACS Meeting. April, 2021. Virtual Oral Presentation.
- “DAT 30: Dative Bonding Benchmark Database”, Southeastern Theoretical Chemistry Association (SETCA). May, 2019. Poster Presentation.
- “Application of Electronic Structure Theory and Machine Learning Methods to Inorganic Chemical Systems”, Candidacy Research Proposal, March, 2020. Oral Presentation.
- “Computational Study of Multi-Nuclear Copper Pyridyl Amide Clusters”, 91st Annual South Carolina Academy of Science Meeting (SCAS). April, 2018. Oral Presentation.
- “Computational Study of Multi-Nuclear Mixed Valence Copper Pyridyl Amide Clusters”, Southeastern Regional American Chemical Society Meeting (SERMACS). October, 2017, Poster Presentation.

WORK EXPERIENCE

2012 - 2016: Terra Firma Landscape Solutions LLC – *Installation Manager*; Lexington, SC

- Hardscape and landscape installation manager
- Customer service – speaking with clients to ensure their vision was coalesced

2016 – 2018: University of South Carolina Aiken – *General Chemistry Stockroom Manager*; Aiken SC

- Digitized MSDS database for all general, organic, and inorganic stockrooms
- Helped in a creating a color-coding system on chemical bottles
- Chemical preparation and quality assurance for general chemistry lab procedures
- Design of various general chemistry lab procedures
- Preparation of stockroom chemical for inorganic lab procedures

2018 – 2022: University of Tennessee Knoxville – *Graduate Teaching Assistant*; Knoxville, TN

- Taught lab and lectures for General chemistry I and II
- Taught lab and lectures for General organic chemistry (precursor to organic chemistry for nursing majors)
- Lecture of selected topics in CHEM 570 (introduction to quantum chemistry and spectroscopy), CHEM 571 (advanced quantum chemistry and spectroscopy), and CHEM 670 (advanced selected topics in physical chemistry).

2018 – 2022: University of Tennessee Knoxville – *Graduate Research Assistant*; Knoxville, TN

- **Research Topics:**
 - Computational catalysis and dynamics
 - Enantioselective aziridination, epoxidation and oxaziridination
 - High-valent Iron(IV) C-H bond activation
 - Mechanistic elucidation of Ring opening metathesis polymerization (ROMP)
 - Electronic structure theory methods
 - Machine learning and molecular representations
- **Responsibilities and Leadership Roles**
 - Team Leader of catalysis collaborations and group projects
 - Lead graduate student for cross-disciplinary collaboration grant proposals
 - Management of group literature exploration

- Management of group purchasing
- **Undergraduate Mentorship:**
 - Katelyn Laughon “Elucidation of Potential Fe(II) Tetracarbene Catalysts for Aziridination Reactions” 2020-2021
 - Elijah Hix “Evaluation of Potential Fe(II) and Cr(II) Tetracarbene Catalysts for Aziridination Reactions” 2020-2021
 - Elokkin Pate-Gaemes “Transition Metal Tetracarbene Mechanistic Approaches for Enantioselective Epoxidation” 2022

HONORS & AWARDS

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| 2013 – 2014 | - 2 x South Carolina Highschool Soccer All State Team |
| 2012 – 2014 | - 3 x South Carolina Highschool Soccer Region IV Team |
| 2016 – 2018 | - USCA Men’s Soccer Team Leader |
| Spring - 2018 | - First Place Outstanding Student Research at the South Carolina Academy of Science Annual Meeting. “Computational Study of Multi-Nuclear Copper Pyridyl Amide Clusters”, 91 st Annual South Carolina Academy of Science Meeting (SCAS). Oral Presentation. |
| 2020 - 2022 | - NIH R15 Research Grant Award “Catalytic Chiral Aziridination with Earth Abundant Metals” |
| 2019 – 2021 | - NSF Chemical Catalysis Research Grant Award “In Silico Design of Molecular Catalysts for C-H Functionalization via Machine Learning Algorithms” |
| 2022 - Present | - NSF Chemical Catalysis Research Grant Award “Chiral Epoxidation and Oxaziridination Catalysis with First-row Transition Metals” |