NATHANIEL LEE KITZMILLER

Department of Chemistry
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EDUCATION

PhD CCQC, University of Georgia, Physical Chemistry with a focus on *ab initio* computational quantum chemistry — May 2024

BS Indiana Wesleyan University, Chemistry — April 2019
Graduated Magna Cum Laude

RESEARCH EXPERIENCE

Assistant Professor of Chemistry
Indiana Wesleyan University, Marion, IN — July 2024 to Present

- Incorporating nonabelian symmetry into a*b initio* electronic structure programs
- Development of reduced cost *ab initio* vibrational analysis methods
- Unimolecular decomposition pathways of low-temperature combustion products

PhD, Research Assistant — November 2019 to Spring 2024
CCQC, University of Georgia, Athens, GA
Advisor: Prof. Henry F. Schaefer III

- *Ab initio* electronic structure, molecular structure method development and applications projects.

Undergraduate Research Assistant — Spring 2017 to Fall 2017
Indiana Wesleyan University, Marion, IN
Advisor: Prof. Scott McCullough

- Used the Force Field Tool Kit (FFTK) to parameterize novel ligand candidates for targeted proteins.

Hodson Summer Research Institute Fellow — Summer 2017
Indiana Wesleyan University, Marion, IN
Advisor: Prof. Scott McCullough

- Used the Force Field Tool Kit (FFTK) to parameterize novel ligand candidates for targeted proteins.

HONORS AND AWARDS

Outstanding TA Award 2024
Awarded for superior teaching skills, as demonstrated through my instructional work at the University of Georgia.

Army Commendation Medal 2023
Award citation: "For exceptional dedication and service while serving as the commander for the 323 Engineer Company located in Spartanburg, SC. First Lieutenant Kitzmiller's leadership contributed greatly to the success of the company's missions from February 2022 to May 2023. First Lieutenant Kitzmiller's actions reflect great credit upon himself, the 323 Engineer Company, and the United States Army."

TEACHING EXPERIENCE

Indiana Wesleyan University, Marion, IN July 2024 to Present
Assistant Professor, Department of Chemistry

- CHE-236L, Organic Chemistry II Lab
- CHE-461, Physical Chemistry Lab
- CHE-440, Physical Chemistry I
- CHE-125, General Chemistry I
- CHE-125L, General Chemistry I Lab
- CHE-235L, Organic Chemistry I Lab
- CHE-450, Physical Chemistry II

University of Georgia, Athens, GA August 2023 to December 2023
Instructor, Department of Chemistry

- CHEM 1210, Basics of Chemistry, an undergraduate lecture-only course averaging 45 students per section, covering chemical principles involving matter, chemical and physical properties, stoichiometry, structure, bonding, and reactivity.

PUBLICATIONS

Peer Reviewed Journal Publications

Kitzmiller, N. L.; Lahm, M. E.; Olive Dornshuld, L. N.; Jincan, J.; Allen W. D.; Schaefer H. F. Convergent Concordant Mode Approach for Molecular Vibrations: CMA-2. *J Chem. Theory Comput.* **2024** *20* (24), 10886-10898

Biggerstaff, S.; Kitzmiller, N. L.; Turney, J. M.; Schaefer, H. F. Comparative Study of Neutral and Cationic Sn_2H_2: Toward Laboratory Detection of the Cation. *J. Phys. Chem. A* **2024** *128* (34), 7090-7104

PUBLICATIONS (CONTINUED)

Goodlett, S. M.; Kitzmiller, N.L.; Turney, J. M., Schaefer H. F. MolSym: A Python Package for Handling Symmetry in Molecular Quantum Chemistry. *J. Chem. Phys.* **2024** *161* (2), 024107.

Lahm, M. E.; Kitzmiller, N. L.; Mull, H. F.; Allen, W. D.; Schaefer H. F. Concordant Mode Approach for Molecular Vibrations. *J. Am. Chem. Soc.* **2022** *144* (51), 23271-23274.

Kitzmiller, N. L.; Wolf, M. E.; Turney, J. M.; Schaefer, H. F. Toward the Observation of the Tin and Lead Analogs of Formaldehyde. *J. Phys. Chem. A* **2022** *126* (43), 7930-7937.

Kitzmiller, N. L.; Wolf, M. E., Turney, J. M.; Schaefer, H. F. The HOX···SO_2 Binary Complexes: Implications for Atmospheric Chemistry. *ChemPhysChem* **2021** *22* (1), 112-126.

CONFERENCE PARTICIPATION

Contributions

PsiCon January 10-11, 2025
Emory University | Atlanta, GA
"Integrating MolSym into Psi4", contributing talk

PsiCon December 8-9, 2023
Georgia Institute of Technology | Atlanta, GA
"The Concordant Mode Approach for Molecular Vibrations", contributing talk

ICQC June 26-July 1, 2023
The Reduta Building | Bratislava, Slovakia
"Extending the Concordant Mode Approach", poster presentation

SETCA May 12-13, 2023
University of South Carolina | Columbia, SC
"Extending the Concordant Mode Approach", poster presentation

MQM June 26-July 1, 2022
Virginia Tech | Blacksburg, VA
"An Extension of the Concordant Mode Approach", poster presentation

LEADERSHIP

Commissioned Officer in the United States Army Reserves 2019 to Present

Current Rank: First Lieutenant
Positions Held:

- Detachment Commander, August 2024 to Present
  316 Psychological Operations Company,
  Peru, IN
- Assistant Operations Officer, June 2023 to July 2024
  HHC, 391st Engineer Battalion,
  Greenville, SC
- Company Commander, February 2022 to May 2023
  323D Engineer Company and 464 Engineer Detachment,
  Spartanburg, SC
- Route Clearance Platoon Leader, May 2020 to January 2022
  323D Engineer Company,
  Spartanburg, SC
- Rear Detachment Commander, December 2019 to April 2020
  323D Engineer Company and 464 Engineer Detachment,
  Spartanburg, SC