# NATHANIEL LEE KITZMILLER

Phone: (260) 403-5999
nate.kitzmiller@indwes.edu
4022 S. Washington St.
Marion, IN 46953

## EDUCATION

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

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

## HONORS AND AWARDS

### *Honors*

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

### *Awards*

**Hodson Summer Research Institute Funding Award** — March 2026
Awarded $22,862 from the Indiana Wesleyan University Hodson Summer Research Institute on March 27th 2026 for the project "Structure-Based Computational Design of SHP-2 Inhibitors."

**Discovered Opportunity Award** — November 2025
Awarded $1000 from the Indiana Wesleyan University Lilly Fund on November 26th 2025 for the project "Increasing the Extensibility of the Concordant Mode Approach"

**Hodson Summer Research Institute Funding Award** — March 2025
Awarded $18,027 from the Indiana Wesleyan University Hodson Summer Research Institute on March 28th 2025 for the project "Reduced-Cost Chemical Kinetics via the Concordant Mode Approach."

**Emerging Faculty Funding Award** — February 2025
Awarded $4000 from the Indiana Wesleyan University Lilly Fund on February 19th 2025 for the project "Reduced-Cost Chemical Kinetics via the Concordant Mode Approach."

## RESEARCH EXPERIENCE

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

## RESEARCH EXPERIENCE (CONTINUED)

- Screening ligand candidates for targeted proteins with QM/MM methods
- Incorporating nonabelian symmetry into *Ab initio* electronic structure programs
- Development of reduced cost *ab initio* vibrational analysis methods
- Unimolecular decomposition pathways of low-temperature combustion products

**PhD** 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** 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** 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.

## TEACHING EXPERIENCE

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

- CHE-104, Chemistry and Artists' Colors
- CHE-104L, Chemistry and Artists' Colors Lab
- CHE-110, Introduction to Chemistry
- CHE-110L, Introduction to Chemistry Lab
- CHE-125, General Chemistry I
- CHE-125L, General Chemistry I Lab
- CHE-235L, Organic Chemistry I Lab
- CHE-236L, Organic Chemistry II Lab
- CHE-330, Inorganic Chemistry
- CHE-440, Physical Chemistry I
- CHE-450, Physical Chemistry II
- CHE-461, Physical Chemistry Lab

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

- CHEM 1210, Basics of Chemistry

## UNIVERSITY SERVICE

**Indiana Wesleyan University**, Marion, IN

Member - University Instructional Technology Council April 2025 to Present

- Encourages and coordinates the use of instructional technology among faculty.
- Promotes activities that will assist faculty with the integration of technology in their teaching and other faculty duties.
- Plans activities and programs for the faculty in coordination with the Vice President of Information Technology to promote the use of instructional technology.
- Advises the university administration with respect to the planning and implementation of changes related to technology, especially as that technology affects teaching and research.

System Administrator – Sisyphus Computer Cluster June 2024 to Present

- Manages the hardware, software, and userbase of the computational computer cluster *Sisyphus* to facilitate student and faculty scholarship and teaching activities.

## PUBLICATIONS

### *Peer Reviewed Journal Publications*

Olive Dornshuld, L.N.; Lahm, M.E.; Kitzmiller, N. L.; Allen, W.D.; Schaefer, H.F. Concordant Mode Approach (CMA): Vibrational Analysis of New and Upgraded Intermolecular Benchmarks for Noncovalent Bonding. *J. Chem. Phys. A* **2026** *130* (16), 3249-3260

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

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.

## PUBLICATIONS (CONTINUED)

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.

## INVITED TALKS

- **Research Seminar** June 30th 2025
  Peter Schreiner Group, Research Seminar
  Justus-Liebig University Giessen, Germany
  "Convergent Concordant Mode Approach for Molecular Vibrations: CMA-2"

## CONFERENCE PARTICIPATION

***Contributions***

- **Winter School of Theoretical Chemistry** December 15-18, 2025
  "Convergent Concordant Mode Approach for Molecular Vibrations: CMA-2"

- **WATOC** January 10-11, 2025
  "Convergent Concordant Mode Approach for Molecular Vibrations: CMA-2"

- **PsiCon** January 10-11, 2025
  "Integrating MolSym into Psi4"

- **PsiCon** December 8-9, 2023
  "The Concordant Mode Approach for Molecular Vibrations"

- **ICQC** June 26-July 1, 2023
  "Extending the Concordant Mode Approach"

- **SETCA** May 12-13, 2023
  "Extending the Concordant Mode Approach"

- **MQM** June 26-July 1, 2022
  "An Extension of the Concordant Mode Approach"

## LEADERSHIP

**Commissioned Officer in the United States Army Reserves** 2019 to Present

Current Rank: Captain
Positions Held:

- Detachment Commander, August 2024 to Present
  A4, 316 Psychological Operations Company,
  Grissom ARB, 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

## REFERENCES

**Jennifer Noseworthy,** Division Chair
Division of Natural Sciences
Indiana Wesleyan University
4021 South Washington Street
Marion, IN 46953
Email: Jennifer.noseworthy@indwes.edu

**Justin Turney**, Senior Research Scientist
CCQC, Department of Chemistry
University of Georgia
140 Cedar Street
Athens, GA 30602
Email: justin.turney@uga.edu

**Henry F. Schaefer**, Graham Perdue Professor of Chemistry
Director, Center for Computational Quantum Chemistry
CCQC, Department of Chemistry
University of Georgia
140 Cedar Street
Athens, GA 30602
Email: ccq@uga.edu