

Zachary J. Knepp

Computational Chemist | PhD Student

 zacharyjknepp |  0000-0002-4382-3205 |  zjk220@lehigh.edu |  U.S. Citizen

Education

Lehigh University

Ph.D. Chemistry

– Chemistry Club VP: Fall 2021, Spring 2022

Bethlehem, PA

Expected Fall 2024

Lock Haven University

B.S. Chemistry and Biology; Minor in Mathematics, *Summa cum Laude*

– Chemistry Club VP: Fall 2020, Spring 2021

Lock Haven, PA

January 2016 – May 2020

United States Army

Basic Combat and 68W (Combat Medic Specialist) MOS Training

Fort Sill, OK and JBSA-Sam Houston, TX

April 2015 – October 2015

Skills

Programming Languages:

Python, Bash, \LaTeX , Mathematica

Computational Chemistry Software:

Gaussian, NWChem, Orca, Dalton, MOLCAS, CRYSTAL, VASP, LAMMPS

Visualization Software:

Gaussview, VESTA, VMD, Avogadro, Blender

Spectroscopy Techniques:

UV-Vis, Fluorescence, Ultrafast Transient Absorption (fitting/analysis)

Misc. Techniques:

Protein Expression, Gel Electrophoresis, Column Chromatography, Assays

Technical Experience

Pennsylvania Army National Guard

Health Care Specialist (68W)

- Performed emergency medical treatments on real and simulated soldiers
- Set up aid-stations and performed outpatient treatments at annual training events and drill weekends
- Provided firing range medical support

Danville, PA

October 2015 - May 2020

Biochemistry Lab Technician

Supervisors: Kyle Root and Jackie Dumm

- Set up lab equipment, prepared various chemical solutions, and tested lab protocols

Lock Haven University

Summer 2017 – Fall 2018

Research Experience

Graduate Research Assistant

Advisor: Lisa Fredin

Lehigh University

Spring 2021 - present

- Executed density functional theory (DFT), time-dependent DFT (TDDFT), and molecular dynamics (MD) simulations of molecules and materials on Lehigh and XSEDE high performance computers (HPC)
- Wrote various Python and Bash programs to automate tasks, process large amounts of data, and generate graphics
- Developed models to approximate the charge carrier mobilities of organic semiconductors with periodic DFT
- Investigated electron-phonon coupling effects in organic crystals with Marcus/Boltzmann transport theories and DFT
- Examined the photo-isomerization and reversion mechanisms of heteroaryl azo dyes with DFT, TDDFT, UV-Vis spectroscopy, and transient absorption spectroscopy in collaboration with Elizabeth Young (Lehigh University)
- Predicted the ground and excited state absorbance spectra of organic and organometallic molecules with linear response, quadratic response, and real-time TDDFT methods in collaboration with Elizabeth Young (Lehigh University)
- Calculated the Raman and IR Spectra of both Organic and Inorganic Materials with DFT calculations in collaboration with Justin Sambur (Colorado State University)
- Determined the reorganization energies of carboxylated $\text{Ru}(\text{bpy})_3$ complexes in various oxidation states with DFT in collaboration with Amanda Morris (Virginia Tech)
- Investigated singlet fission materials with varying substituents and packing arrangements with DFT and LR-TDDFT calculations in collaboration with NIST and John Anthony (University of Kentucky)

Undergraduate Research Assistant

Advisor: Kevin Range

Lock Haven University

Spring 2020

- Mastered the basics of the Linux command line
- Ran NVT and NPT molecular dynamics (MD) simulations on Comet supercomputers
- Investigated the dynamics of an M37 lipase protein in TIP3P water and in a POPC bilayer with AMBER force-fields and software

Undergraduate Research Assistant

Advisor: Kyle Root

Lock Haven University

Spring 2018 – Summer 2019

- Performed kinetic studies using a novel ester substrate of a lipase protein sourced from rice bran
- Identified and partially purified an uncharacterized esterase from *Aphanizomenon flos-aquae*, using an ammonium sulfate precipitation and hydrophobic interaction chromatography
- Recombinantly expressed hypA (Nickel binding protein) in *Escherichia coli* in the presence of $\text{NiSO}_4 \cdot 6 \text{H}_2\text{O}$ to investigate Nickel tolerance based forced gene expression
- Developed an on-column refolding protocol for recombinantly expressing esterase from inclusion bodies using Empigen BB Detergent
- Characterized recombinantly over-expressed thermophilic lipase native to *Sphaerobacter thermophilus* and a psychrophilic esterase native to *Aphanizomenon flos-aquae*

Teaching and Mentoring Experience

Quantum Chemistry Workshop Teaching Assistant

Instructor: Lisa Fredin

Lehigh University

Summer 2021, Summer 2022, Summer 2023

- Assisted students with executing Linux commands, command-line text editor (e.g. Vim) usage, and SLURM scripting for high-performance computing (HPC)
- Helped students prepare input files and SLURM scripts for running molecular DFT jobs on HPCs with Gaussian and Gaussview software
- Aided students in constructing unit- and super-cells of simple periodic solids for Quantum ESPRESSO based DFT jobs

Photochemistry Undergraduate Research Experience Mentor

Advisors: Lisa Fredin and Elizabeth Young

Lehigh University

Summer 2021 - present

- Mentored 8 undergraduate students in best practice computational chemistry, data processing, and graphical design
- Taught and reviewed aspects of photochemistry, quantum mechanics, and DFT to students with a general chemistry background
- Provided feedback on writing, presentation preparation and execution, and project progression
- Designed step-by-step tutorials for complicated computational procedures

CHM 341: Molecular Structure, Bonding, & Dynamics Guest Lecturer

Instructor: Lisa Fredin

Lehigh University

Spring 2023

- Lecture 1: Quantum mechanics overview, particle-in-a-box, superposition of states, and the uncertainty principle
- Lecture 2: Multi-electron atoms, the variational theorem, and the self-consistent-field Hartree-Fock method
- Adapted slides and course material

CHM 343: Physical Chemistry Lab Teaching Assistant

Instructor: Elizabeth Young

Lehigh University

Spring 2022

- Set-up and co-instructed physical chemistry labs to ≈ 34 students
- Graded lab reports and provided feedback and comments
- Assisted in the development of Mathematica data-processing scripts

CHM 030: General Chemistry Lab Teaching Assistant

Instructors: Hannah Cronk, Daniel Prendergast, and Cynthia Velgus

Lehigh University

Fall 2020, Spring 2021

- Taught weekly pre-labs to ≈ 18 students across 2 sections
- Supervised experimental set-up and execution
- Graded ≈ 36 lab reports weekly
- Held office hours every other week to assist students with their lab reports

Mathematics Tutor

Supervisor: Jacinth Maynard

Lock Haven University

Fall 2019, Spring 2020

- Provided tutoring for students in Algebra, Calculus I, and Calculus II
- Assisted students with homework problems and test preparations

Outreach

STEM Outreach at Pre-K Daycares

Volunteer

- Traveled 6 times to conduct hands-on science experiments with \approx 20 pre-K children
- Prepared and tested a variety of age appropriate science experiments

Bethlehem, PA

Fall 2022 – Summer 2023

Workshops and Events

TDDFT School & Workshop: Excited States and Dynamics

Sponsor: Rutgers University - Newark

Newark, NJ

Summer 2023

- Attended theory lectures, hands-on activities, hackathons, and presented at two poster sessions on applications of TDDFT

Solid State Materials Chemistry & Data Science Hackathon

Sponsors: NSF, University of Utah, and Lehigh University

Bethlehem, PA

Winter 2023

- Assisted in the development of a Python-based epitaxial matching software

Honors and Awards

Spring 2024 CAS Dean's Research Fellowship at Lehigh University

Summer 2019 Opportunity Award for Research (SOAR) Scholars Award at Lock Haven University

Summer 2018 Opportunity Award for Research (SOAR) Scholars Award at Lock Haven University

2018 Rose Witt Kleinman Memorial Scholarship at Lock Haven University

Publications

4. Martin, S. M.; **Knepp, Z. J.**; Thongchai, I. A.; Englehart, K.; Sorto, K.; Jaffer, A.; Fredin, L. A.; Young, E. R. The Doorstop Proton: Acid-controlled Photoisomerization in Pyridine-Based Azo Dyes. *New Journal of Chemistry* **2023**, 47, 11882–11889.
3. **Knepp, Z. J.**; Masso, G. B.; Fredin, L. A. Efficiently predicting directional carrier mobilities in organic materials with the Boltzmann transport equation. *The Journal of Chemical Physics* **2023**, 158, 064704.
2. **Knepp, Z. J.**; Fredin, L. A. Real temperature model of dynamic disorder in molecular crystals. *The Journal of Physical Chemistry A* **2022**, 126, 3265–3272.
1. **Knepp, Z. J.**; Ghaner, A.; Root, K. T. Purification and refolding protocol for cold-active recombinant esterase AaSGNH1 from *Aphanizomenon flos-aquae* expressed as insoluble inclusion bodies. *Preparative Biochemistry & Biotechnology* **2021**, 52, 394–403.

Manuscripts in Progress

6. **Knepp, Z. J.**; Repa, G. M.; Fredin, L. A. Modeling Excited States from Molecules to Materials (Review). *In preparation*.
5. Chen, A. H.; **Knepp, Z. J.**; Fredin, L. A. On the sterically hindered indole-based azo dyes photoisomerization and reversion mechanisms. *In preparation*.
4. **Knepp, Z. J.**; Hamburger, R. C.; Thongchai, I. A.; Englehart, K.; Sorto, K.; Jaffer, A.; Young, E. R.; Fredin, L. A. Protons restrict the photoisomerization of pyridine-based azo dyes on ultrafast timescales. *In preparation*
3. **Knepp, Z. J.**; Fredin, L. A. Finite Displacement Boltzmann Transport Theory (Δ BTE) Reveals the Detrimental Effects of High Frequency Phonons on Mobility. *In review*.
2. Repa, G. M.; **Knepp, Z. J.**; Fredin, L. A. A-site doping to alter oxygen mobility in SrTiO₃. *In review*.
1. Thongchai, I. A.; **Knepp, Z. J.**; Fertil, D. R.; Flynn, H.; Young, E. R.; Fredin, L. A. Acid Violet 3: A Base Activated Water-Soluble Photoswitch. *Accepted*.

Posters and Presentations

10. **Knepp, Z. J.**; Young, E. R.; Fredin, L. A. Investigating the Photoisomerization Mechanisms of Hetero-aryl Azo Dyes with Theory and Experiment, **2023**, Poster present at the Photochemistry Gordon Research Conference, Lewiston, ME.
9. **Knepp, Z. J.**; Fredin, L. A. Computational Pump-Probe Spectra for Free with LR-TDDFT, **2023**, Poster presented at Rutgers University-Newark's TDDFT School and Workshop, Newark NJ.

8. Howzen, A.; Repa, G. M.; **Knepp, Z. J.**; Pimputkar, S.; Strandwitz, N. C.; Fredin, L. A. Data driven interface design, **2023**, Poster presented at Institute for Data, Intelligent Systems, and Computation, Lehigh University, Bethlehem PA.
7. **Knepp, Z. J.**; Fredin, L. A. Modeling Dynamic Disorder in Organic Materials, **2022**, Poster presented at the Mid-Atlantic Regional ACS Meeting, Ewing, NJ.
6. Elliott, K. A.; **Knepp, Z. J.**; Ostrander, H.; Hogan, S.; Root, K. T. Lock Haven University Chemistry Club, **2019**, Poster presented at the American Chemical Society National Meeting, Orlando, FL.
5. **Knepp, Z. J.**; Ghaner, A.; Root, K. T. Characterization of a Psychrophilic Esterase from Blue-Green Algae, **2019**, Poster presented at the LHU Celebration of Scholarship, Lock Haven, PA.
4. **Knepp, Z. J.**; Sutton, M. M.; Root, K. T. Characterization of a Thermophilic Lipase from *Sphaerobacter thermophilus*, **2019**, Poster presented at the 59th Annual Natural Sciences Convocation, Lock Haven, PA.
3. **Knepp, Z. J.**; Sutton, M. M.; Root, K. T. Characterization of a Thermophilic Lipase from *Sphaerobacter thermophilus*, **2019**, Poster presented at the Penn State Undergraduate Research Symposium, State College, PA.
2. **Knepp, Z. J.**; Root, K. T. Development of a Novel Detergent-Free Lipase Assay, **2018**, Poster presented at the LHU Celebration of Scholarship, Lock Haven, PA.
1. **Knepp, Z. J.**; Root, K. T. Purification of an Esterase from *Aphanizomenon flos-aquae*, **2018**, Poster presented at the Penn State Undergraduate Research Symposium, State College, PA.