WOOK SHIN

800 19th Avenue S. Nashville TN, 37203, USA | 512-826-0572 | wook.shin@vanderbilt.edu | Office: MRB III 5154F

EDUCATION

Vanderbilt University **May 2026 Expected**
- Ph.D. program in Department of Chemistry

Vanderbilt University **Degree Conferred 2023**
- Master of Science in Chemistry

University of California, Los Angeles (UCLA) **Degree Conferred 2020**
- Bachelor of Science in Chemistry
  - Physical Chemistry Concentration | Specialization in Computing

PUBLICATIONS

- **Wook Shin**, Xinchun Ran, Zhongyue J. Yang*. "Accelerated Entropic Path Sampling with a Bidirectional Generative Adversarial Network" The Journal of Physical Chemistry B 2023 127 (19), 4254-4260
- **Wook Shin**, Zhongyue J. Yang*. "Computational Strategies for Entropy Modeling in Chemical Processes." Chem. Asian J. 2023, e202300117
- Erik P. Farr*, Jason C. Quintana, Vanessa Reynoso, Josiah D. Ruberry, **Wook R. Shin**, and Kevin R. Swartz. "Introduction to Time-Resolved Spectroscopy: Nanosecond Transient Absorption and Time-Resolved Fluorescence of Eosin B." Journal of Chemical Education 2018 95 (5), 864-871

RESEARCH EXPERIENCE

ZJYang Research Group, Vanderbilt University **Nashville, TN**
GRADUATE RESEARCH ASSISTANT | Advisor: Dr. Zhongyue J. Yang *August 2021 to Present*
- Conduct research in the field of computational chemistry, with a primary focus on advancing thermodynamic path sampling techniques for characterizing the energetics, entropies, kinetics, and selectivity of chemical processes.
- Developed the **Bidirectional Generative Adversarial Network-Entropic Path Sampling** protocol, designed to expedite configurational entropy calculations by substantially reducing the number of molecular dynamics simulation trajectories required (from ∼2000 trajectories to ∼100 trajectories)
- Conceptualized and curated benchmark datasets for enzyme classifications, accompanied by experimental kinetics data, to support the creation of Enzyme-RosettaQM.

Neuhauser Research Group, UCLA **Los Angeles, CA**
UNDERGRADUATE RESEARCH ASSISTANT | Advisor: Dr. Daniel Neuhauser *September 2015 to February 2021*
- Studied **time-dependent quantum-mechanical methods for molecular dynamics calculations** in Fortran 90.
- Implemented numerical methods such as Euler method, Chebychev propagation, Verlet integration, second-order differencing, and evolution and split operators.

Physical Chemistry Laboratory (Honors), UCLA **Los Angeles, CA**
UNDERGRADUATE RESEARCH ASSISTANT *April 2017 to October 2017*
- Co-authored "Introduction to Time-Resolved Spectroscopy: Nanosecond Transient Absorption and Time-Resolved Fluorescence of Eosin B" **(J. Chem. Educ. 2018, 95, 5, 864-871)**.
- Contributed to the design of an undergraduate upper division laboratory experiment that introduced the concepts of time-resolved spectroscopy and photochemistry.
- Designed an experiment extension for the investigation of heavy-atom effect via nitrogen gas quenching process.

PRESENTATIONS AND POSTER SESSIONS

- American Chemical Society Fall 2023 Symposium Presentation
  - Deep Learning-Generated Free Energy Profiles for Chemical Reactions
- Houk Research Conference 2022 Presentation
  - Bidirectional Generative Adversarial Network for Evaluating Entropic Profile from Reaction Dynamic Trajectories
- American Conference on Theoretical Chemistry (ACTC) 2022 Poster Session
  - Bidirectional Generative Adversarial Network for Evaluating Entropic Profile from Reaction Dynamic Trajectories

WORK EXPERIENCE

Department of Chemistry, Vanderbilt University **Nashville, TN**
Graduate Teaching Assistant *August 2021 to Present*
- Provide lectures to students in General Chemistry I Lab, Physical Chemistry Lab, and Biophysical Chemistry Course.
- Took charge of autonomous classroom instruction, including proctoring exams, implementing the lesson plans set by the professors and grading assignments.

SHIN-A T&C Carbon Nanotube (CNT) & Graphene Research Division **Seoul, South Korea**
Research Intern *February 2021 to July 2021*

- Conducted experimental studies on the reaction mechanisms involved in the dispersant-free dispersion of multi-walled carbon nanotubes, specifically focusing on Carbon Nanotube-Quadruple Hydrogen Bonding (CNT-QHB) synthesis. Designed and optimized a procedure to reduce the synthesis time from 72 hours to 24 hours."
- Produced carbon nanotube (CNT) dispersed products for various applications, including batteries, displays, and waterproof coatings, utilizing high-pressure homogenizers, multi-force dispersers, ball-milling, and other manufacturing methods.

California NanoSystems Institute(CNSI) Education Outreach Program **Los Angeles, CA**
UNDERGRADUATE OUTREACH INTERN *September 2020 to December 2020*

- Collaborated in the organization of laboratory experiment kits and facilitated the creation of computational workshops designed for remote educational engagement in response to the COVID-19 pandemic.

Republic of Korea Army (ROKA) Division 39 Regiment 118 Battalion 2 **Namhae, South Korea**
RADAR OPERATOR, SERGEANT *July 02 2018 to February 22 2020*

- Operated radars to monitor and track over 120 ship activities across four distinct surveillance sites.
- Devised a Visual Basics program that facilitated the execution of sea state code, operation area checks, and tracking reports.
- Recognized by Operation Commander for detecting a sinking boat and collaborating with the Korea Coast Guard to rescue two drifters.
- Graduated at the top of the class (1st out of 80+) from the ROK Army Signal School and instructed more than 50 prospective radar operators.

AMEP, High-Tech Plant Electrical Design **Dongtan, South Korea**
INTERN *July 2014 to September 2014*

- Participated in The Samsung Semiconductor Plan Retrofit Project and The Electrical Plan Modification Project, ensuring successful project completion through diligent efforts.
- Developed a Python program to modify electrical plan data formats and identify blueprint modifications, enabling the creation of an Integrated Database Management System.

HONORS AND AWARDS

- 2021 Tarbell/Warren Fellowships - Departmental Graduate Award — Vanderbilt University
- UCLA Dean's List S2020, F2020 — UCLA
- Second Operational Command General Recognition Award — ROKA
- ROK Army Signal School Recognition Award — ROKA

TECHNICAL SKILLS

- **Computational Methods:** Configurational Entropy Calculation, Deep Learning/Generative Model, Molecular Dynamics, Monte Carlo and Quantum Mechanics/Molecular Mechanics (QM/MM) simulations
- **Programming Languages:** Python, Fortran90, C++, Gaussian09, AutoCAD, R, Visual Basic, MATLAB, LabView, Octave, and LaTeX
- **Languages:** English and Korean (native)

CERTIFICATION

- Coursera: Machine Learning — October 27 2020