Kun-Lin (Calvin) Wu

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SUMMARY

A research scientist with a passion in using data to solve real-world problems. 5+ years of research experience specializing in quantum simulation and machine learning for material developments, including catalysts for carbon capture and battery materials. Collaborated with scientists from universities, national labs and energy companies. Experienced in teaching, presentations and scientific publications. Strived to contribute cutting-edge discoveries through data-driven innovations.

EDUCATION

Ph.D. in Chemical Engineering, University of California Davis, CA **expected June 2025**

- Provisional thesis title: The kinetics and dynamics of CO_2 adsorption in zeolite material under humid environment
- Relevant classes: ECS 271- machine learning and discovery; ECS 289- advanced deep learning

M.S. in Chemical Engineering, University of Washington, WA **June 2020**

- Dissertation title: Pharmacological Regulation of Protein-Polymer Hydrogel Stiffness

B.S. in Chemical Engineering, National Taiwan University, Taipei **June 2017**

RESEARCH EXPERIENCES

Graduate Student Researcher **September 2020 - Present**

University of California, Davis, California | Advisor: Ambarish Kulkarni

- Developed a theory and numerical implementation for modeling CO_2 adsorption in catalyst under humid condition.
- Designed and developed data workflows to automate simulations on HPC system.
- Analyzed and visualized molecular dynamic simulations using python to validate experiment observations.
- Trained and fine-tuned deep learning models by evaluating the model prediction for molecule interactions.
- Applied machine learning models to scale up molecular dynamic simulation to real-world timescale.

Quantum Simulations Group, Lawrence Livermore National Lab **January 2024 – June 2024**

Research Assistant | Advisor: Sabrina Wan

- Developed models for electrode material to study lithium de-solvation process at the electrolyte-electrode interface.
- Created 20+ electrode material models selectively and visualized the models through pymatgen and VESTA software.
- Performed theory calculations and simulations on HPC to evaluate electrode material stability.

University of Washington, Seattle, Washington **September 2018 - July 2020**

Graduate Student Researcher | Advisor: Cole DeForest

- Employed protein engineering and molecular biology to design and synthesize biomaterials for drug delivery.
- Performed elemental analysis and characterized the mechanical properties of materials.

PUBLICATIONS

- Lee, H., ***Wu, K. L. (co-first),*** Xie, D., Xu, L., Okrut, A., Zones, S. I., ... & Katz, A. (2024). Understanding Water Enhancement of CO2 Adsorption in Zeolite Cs–RHO. Chemistry of Materials.
  Selected as a front cover for the journal
- ***Wu, K. L.,*** Bretherton, R. C., Davis, J., & DeForest, C. A. (2023). Pharmacological regulation of protein-polymer hydrogel stiffness. RSC advances, 13(35), 24487-24490.
- Xu, L., Okrut, A., Tate, G. L., Ohnishi, R., ***Wu, K. L.,*** Xie, D., ... & Katz, A. (2021). Cs-RHO goes from worst to best as water enhances equilibrium CO2 adsorption via phase change. Langmuir, 37(47), 13903-13908.

TECHNICAL SKILLS

- **Programming and Software**: Python, Git/GitHub, Jupyter Notebook
- **High Performance Computing (HPC)**: Shell script, parallel programming (MPI libraries)
- **Machine learning**: Scikit-learn, TensorFlow, PyTorch, MACE
- **Scientific Computing:** Density Functional Theory (DFT) Calculations (VASP, Quantum ESPRESSO)

CONFERENCES PRESENTATIONS

- ***Wu, K. L.*** (Fall 2023). "Why does Cs-RHO show increased CO_2 uptakes in the presence of water?" American Chemical Society (ACS) Meeting.
- ***Wu, K. L.*** (Spring 2023). "Enabling Rigorous Quantification of Humid CO_2 Adsorption/Desorption in Zeolites". Center for Rational Catalyst Synthesis (CERCAS) Meeting.
- ***Wu, K. L.*** (Spring 2022). "CO_2 adsorption/desorption from zeolites under humid environments". Center for Rational Catalyst Synthesis (CERCAS) Meeting.

HONORS AND AWARDS

- **RSC Advances Outstanding Student Paper Awards**- Materials Chemistry, 2023.
- **Honorable Mention Recipient**, NTU Innovative Chemical Process Design Contest, April 2016

WORKSHOPS

- **NERSC GPU Hackathon**, August 2024.
- **Deep Modeling for Molecular Simulation Workshop,** Princeton University, July 2022.

TEACHING EXPERINECES

University of California, Davis, California **March 2021 - June 2022**

Teaching Assistant

- Prepared course materials with the instructor and lectured on Python programming for engineering problems.
- Facilitated and led group discussions on Python problems and thermodynamics topics.
- Planned lessons and assignments, hold office hours and graded papers and exams.
- Classes: Engineering Problem Solving using Python, Thermodynamics

University of Washington, Seattle, Washington **September 2019 - June 2020**

Teaching Assistant Lead

- Instructed a class of 48 senior students on molecular biology lab techniques independently.
- Collaborated with professors to facilitate a general biology course for over 800 undergraduate students.
- Assessed laboratory reports, graded exams, conducted office hours, and developed online course materials.
- Classes: Laboratory Techniques in Cell and Molecular Biology, Introductory Biology

PROFESSIONAL SERVICE

UC Davis Chemical Engineering Graduate Student Organization **September 2021 – June 2022**

Alumni/ Industry Chair

- Organized industry panels to create networking between students and alumni.
- Collaborated with faculty and student leaders to align events with students' career goals and industry trends.

National Taiwan Science Education Center, Taipei **June 2017 – June 2018**

Military Service

- Organized and managed the 57th National Science Poster Contest and facilitated participation from elementary to high school students across Taiwan.
- Designed and conducted experiments while mentoring students in poster creation to inspire interest in science among elementary to high school students.

Office of International Affairs, National Taiwan University, Taipei **September 2015 – July 2016**

NTU Student Ambassador

- Collaborated with staff and ambassadors to organize and coordinate three international research conferences.
- Assisted 50+ scholars from international institutions, providing support for travel and accommodations.

REFERENCES

Ambarish Kulkarni, Associate Professor
Department of Chemical Engineering
University of California, Davis
Email: arkulkarni@ucdavis.edu

Liwen (Sabrina) Wan, Staff Scientist
Quantum Simulation Group
Lawrence Livermore National Laboratory
Email: wan6@llnl.gov