Hoang (Bolton) Tran, Ph.D.

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Education

Pennsylvania State University, Ph.D. in Chemical Engineering — Sept 2018 – Aug 2023
Thesis: Electrocatalysis at the Electrode/Electrolyte Interface: a Multiscale Molecular Model

Drexel University, B.S. in Chemical Engineering — Sept 2012 – June 2017

Research

Postdoctoral Research Fellow—*University of Michigan, Ann Arbor, MI* — Sept 2023 – present
Advisor: Prof. Bryan R. Goldsmith

- Developing machine learning methods for the discovery of materials in electrochemical applications.
- Investigating vanadium-based batteries with quantum chemistry and machine-learning interatomic potentials.
- Developed machine learning frameworks for predicting anion adsorption on electrodes.
- Elucidated the effects of electrochemical voltage on the kinetics of CO_2 reaction.
- Train and mentor 3 doctoral students and 4 undergraduate students in their research activities.

Doctoral Research Assistant—*Pennsylvania State University, University Park, PA* — Sept 2018 – Aug 2023
Advisors: Prof. Michael J. Janik & Prof. Scott T. Milner

- Developed molecular dynamics method to investigate water and ions at the solid-liquid interfaces.
- Advanced understanding of organic solvents' impact on biomass reaction kinetics.
- Co-authored a book chapter on the application of density functional theory in electrocatalysis research.
- Trained and mentored 2 undergraduate students resulting in peer-reviewed publications.

Undergraduate Research Assistant—*Drexel University, Philadelphia, PA* — Sept 2014 – Apr 2015
Advisors: Prof. Jason Baxter

- Developed chemical deposition techniques for solar cell fabrication.

Teaching

Atomistic scale simulations, ME/CHE 505, Pennsylvania State University — Spring 2022
Guest lecturer (six one-hour lectures)

Simulation techniques and applications, CHE 597, Pennsylvania State University — Fall 2022
Guest lecturer (an one-hour lecture)

Material balance, CHE 210, Pennsylvania State University — Fall 2022
Graduate teaching assistant (in-person, flipped classrooms)

Reaction engineering, CHE 430, Pennsylvania State University — Spring 2021
Graduate teaching assistant (virtual office hours, in-person exam reviews)

Research Mentoring

Pennsylvania State University

- Elizabeth Long, Women In Science and Engineering Research (WISER) undergraduate researcher
- Yusheng Cai, undergraduate researcher, now a Ph.D. candidate at the University of Pennsylvania
- Joe Hughes, undergraduate researcher, now an engineer at Naval Reactors

University of Michigan

- Ankit Mathanker, 4th year Ph.D. candidate
- Dean Sweeney, 2nd year Ph.D. candidate
- Roshini Dantuluri, 2nd year Ph.D. candidate
- Yifei Liu, undergraduate researcher
- Mad Lindsey, undergraduate researcher
- Jean-Pattrick Selo, community college researcher

Publications

Published peer-reviewed papers

1. Long, E., **Tran**, **B.**, Milner, S. T., "Tuning partial charges of alkyl alcohols to improve simulated fluid properties", J. Chem. Phys. **162** (2025)
2. **Tran**, **B.**, Janik, M. J., Milner, S. T., "Hydration-Shell Solvation and Screening Govern Alkali Cation Concentrations at Electrochemical Interfaces", J. Phys. Chem. C **128**, 20559–20568 (2024)
3. Mathanker, A., Halarnkar, S., **Tran**, **B.**, Singh, N., Goldsmith, B. R., "Synergistic effects in organic mixtures for enhanced catalytic hydrogenation and hydrodeoxygenation", Chem Catal., 101135 (2024)
4. **Tran**, **B.**, Goldsmith, B. R., "Theoretical Investigation of the Potential-Dependent CO Adsorption on Copper Electrodes", J. Phys. Chem. Lett. **15**, 6538–6543 (2024)
5. Wong, A., **Tran**, **B.**, Agrawal, N., Goldsmith, B. R., Janik, M. J., "Sensitivity Analysis of Electrochemical Double Layer Approximations on Electrokinetic Predictions: Case Study for CO Reduction on Copper", J. Phys. Chem. C **128**, 10837–10847 (2024)
6. **Tran**, **B.**, Zhou, Y., Janik, M. J., Milner, S. T., "Negative Dielectric Constant of Water at a Metal Interface", Phys. Rev. Lett. **131**, 248001 (2023)
7. Ostervold, L., Daneshpour, R., Facchinei, M., **Tran**, **B.**, Wetherington, M., Alexopoulos, K., Greenlee, L., Janik, M. J., "Identifying the Local Atomic Environment of the "Cu3+" State in Alkaline Electrochemical Systems", ACS Appl. Mater. Interfaces **15**, 27878–27892 (2023)
8. **Tran**, **B.**, Milner, S. T., Janik, M. J., "Kinetics of Acid-Catalyzed Dehydration of Alcohols in Mixed Solvent Modeled by Multiscale DFT/MD", ACS Catal. **12**, 13193–13206 (2022)
9. **Tran**, **B.**, Cai, Y., Janik, M. J., Milner, S. T., "Hydrogen Bond Thermodynamics in Aqueous Acid Solutions: A Combined DFT and Classical Force-Field Approach", J. Phys. Chem. A **126**, 7382–7398 (2022)
10. Edley, M. E., Opasanont, B., Conley, J. T., **Tran**, **H.**, Smolin, S. Y., Li, S., Dillon, A. D., Fafarman, A. T., Baxter, J. B., "Solution processed CuSbS2 films for solar cell applications", Thin Solid Films **646**, 180–189 (2018)

Manuscripts in revision, submission, or preparation

1. Sweeney, D., **Tran, B.**, Goldsmith, B. R., "Potential Dependence of Nitrate Adsorption and Dissociation across Metals and Dilute Alloys: a Grand Canonical Study", manuscript in revision.
2. **Tran, B.**, Goldsmith, B. R., "Predicting Competitive Anion Electrosorption on Late Transition Metals", manuscript submitted.
3. Manthanker, A., Sharma, G., **Tran, B.**, Signh, N., Goldsmith, B. R., "Effect of Ions on the Aqueous-Phase Adsorption of Benzene, Phenol, and Catechol on Ag(111)", manuscript submitted.
4. **Tran, B.**, Sweeney, D., Selo, J., Liu, Y., Lindsey, M., Goldsmith, B. R., "Effects of hydration on the predictive power of O-H stretching frequency on acid pKa", manuscript in preparation.

Conference Presentation

- **North American Catalysis Society 2025 (expected)** | Atlanta | oral & poster presentations.
- **American Institute of Chemical Engineering Annual Meeting 2024** | San Diego | oral & poster presentations.
- **American Chemical Society Fall Meeting 2024** | Denver | oral & poster presentations.
- **Gordon Research Seminar/Conference 2024** | New London | oral (invited) & poster presentations.
- **Michigan Catalysis Society 2024** | Ann Arbor | oral presentation.
- **American Chemical Society Spring Meeting 2023** | Indianapolis | oral presentation.
- **American Institute of Chemical Engineering Annual Meeting 2022** | Phoenix | oral & poster presentations.
- **Pittsburgh-Cleveland Catalysis Society 2022** | State College | poster presentation.
- **North American Catalysis Society 2022** | New York | oral & poster presentations.
- **American Chemical Society Spring Meeting 2022** | Virtual | oral presentation.
- **American Physical Society March Meeting 2022** | Chicago | oral presentation.
- **American Institute of Chemical Engineering Annual Meeting 2021** | Boston | oral presentation.

Industry

Quality Assurance Associate—*Avid Radiopharmaceuticals, Philadelphia, PA* Nov 2016 – Aug 2018

- Supported the quality control for the production of Amyvid, a radiotracer drug for Alzheimer's disease.

Analytical Chemistry Intern—*Zeolyst International, Conshohocken, PA* May 2014 – Sept 2014

- Analyzed zeolites for the Selective Catalytic Reduction process in catalytic converters.

Skills

- Quantum Chemistry: Gaussian, VASP, JDFTx, NWChem
- Molecular Dynamics: GROMACS, LAMMPS
- Machine Learning: Scikit-learn, RDKit, TensorFlow, SISSO
- Programming: Python, C++, VBA, SQL, HTML/CSS, Bash, Git
- Chemistry Databases: Materials Project, Open Catalysis, CCCBDB
- Documentation and Visualization: LaTeX, Matplotlib, Plotly, ASE, VMD

Awards

- University of Michigan postdoctoral travel award | American Chemical Society Fall Meeting 2024
- ACS CATL ChemCatBio travel award | American Chemical Society Spring Meeting 2023
- Poster presentation 1st place | Pittsburg-Cleveland Catalysis Society 2022
- FGSA travel award | American Physical Society March Meeting 2022
- Departmental best qualifying exam | Pennsylvania State University 2019

Broader Impact Activities

- Poster-judged for University of Michigan's Undergraduate Research Annual Symposium, 2025.
- Volunteered session-chair at the Midwest Thermodynamics and Statistical Mechanics Conference, 2024.
- Poster-judged for University of Michigan Graduate Research Symposium, 2023.
- Founded and led a Vietnamese Graduate Student Association at Pennsylvania State University, 2022.