KEVIN TRAN

Curriculum Vitae ◇ Updated on 2025 August 07

Toyota Research Institute ◇ Energy & Materials ◇ Accelerated Materials Discovery & Design

EDUCATION

Carnegie Mellon University *2016–2021*
PhD in Chemical Engineering
University of Delaware *2007–2011*
Bachelor's of Science in Chemical Engineering, Minor in Philosophy

EMPLOYMENT HISTORY

2024–Present	**Staff Research Scientist**, Toyota Research Institute, Energy & Materials
2022–2024	**Senior Research Scientist**, Toyota Research Institute, Energy & Materials
2021–2022	**Senior Scientist**, Schrödinger, Materials Science Department
2016–2021	**Graduate Research Assistant**, Carnegie Mellon University, Chemical Engineering
2019	**Intern**, Lawrence Livermore National Lab, Quantum Simulations Group
2014–2016	**Process Engineer**, W.L. Gore & Associates, Bioresorbable Polymers
2011–2014	**Process Engineer**, W.L. Gore & Associates, PTFE Paste Processing
2010–2011	**Intern**, W.L. Gore & Associates, Fuel Cell Electrodes
2009–2010	**Tutor**, University of Delaware, Office of Academic Enrichment
2009	**Intern**, W.L. Gore & Associates, Steam Sterilization
2007–2009	**Lab Assistant**, University of Delaware, Institute of Energy Conversion

WORK & RESEARCH EXPERIENCE

Staff Research Scientist Toyota Research Institute, Remote
Causal learning of electrochemical systems *November 2024–Present*

· Leading a causal learning research strategy. Using the strategy to accelerate the discovery of fundamental insights for sustainable electrochemical technologies—e.g., fuel cells or batteries. Focusing the strategy on industrial research gaps to mitigate business risk, while also benchmarking against other state-of-the-art AI methods to monitor research risk.

Senior Research Scientist Toyota Research Institute, Remote
Autonomous laboratory development *July 2022–November 2024*

· Helped direct a cross-functional team of researchers and engineers across two universities and two companies. Guided the team to create a fully automated self-driving-laboratory. Used the self-driving laboratory to develop new active learning methods tailored to probe material and device stability, aimed at ultimately discovering long-lasting catalysts.

· Mentored and trained several industrial and academic researchers. For example: Trained machine learning researchers on project management and software engineering practices, helping them grow a deep learning team. Also trained graduate students in statistical design of experiments and analysis of variance. Ultimately accelerated their ability to derive fundamental understanding of fuel cell catalysts.

Senior Scientist Schrödinger, New York NY
Materials science development *April 2021–July 2022*

- Led the initial design and development of a microkinetic modeling package. This served as the foundation for a new product line that connected density functional theory calculations to experimentally measurable quantities—e.g., concentration profiles.
- Accelerated research and development of surface chemistries by creating and maintaining software that performed, managed, and analyzed atomic-scale simulations (e.g., molecular dynamics or density functional theory calculations).

Graduate Research Assistant Carnegie Mellon University, Pittsburgh PA
Chemical Engineering *August 2016–January 2021*

- Participated in the founding of the Open Catalyst Project (OCP), a collaboration between Facebook's AI Research group and Carnegie Mellon University. Via OCP, we outlined and implemented a path to accelerate the creation of a sustainable energy economy by using high performance computing and machine learning to discover catalysts.
- Collaborated with several institutions across multiple projects to find catalysts to create sustainable solar fuels and solar chemicals. Provided experimental partners with high-value candidate catalysts by creating and managing an end-to-end data science framework that performs high-throughput Density Functional Theory (DFT) calculations. Combined the framework with active machine learning methods to create a fully automated algorithm for discovering new materials. Managed all code, results, analyses, and databases in an open-source environment.
- Used the end-to-end framework to aid collaborators in experimentally discovering a new catalyst with record-breaking selectivity for ethylene production. Used the same framework to aid different collaborators in experimentally discovering a new catalyst for hydrogen evolution.
- Helped manage a new research group as the first PhD student. Assisted in conception and writing of various grants and proposals. Defined and implemented a training regimen for new group members to learn the basics of project management, catalysis, programming, machine learning, and software development. Helped successfully grow the group from 2 members to ∼20 fully funded members.

Intern Lawrence Livermore National Lab, Livermore CA
Computational Chemistry and Materials Science Institute *June 2019–August 2019*

- Worked with the Quantum Simulations Group to optimize processing conditions for electrochemical solar fuel and chemical production.
- Accounted for previously overlooked processing conditions such as solvent, electrolyte, and voltage by implementing and automating novel DFT simulation methods.

Process Engineer W.L. Gore & Associates, Elkton MD
Bioresorbable polymer synthesis *August 2014–July 2016*

- Initiated and led a project to model polymer synthesis processes on both lab-scale and production-scale, enabling faster development/scale-up time of new products and faster trouble-shooting for product manufacturing.
- Used the aforementioned model to reduce production yield losses by 30%. Implemented all changes in an FDA-regulated environment while simultaneously overseeing day-to-day manufacturing.

Process Engineer W.L. Gore & Associates, Elkton MD
PTFE paste processing and expansion *August 2011–July 2014*

- Enabled faster process development time for a broad range of implantable medical devices by designing, executing, and documenting experiments to gain fundamental understanding of process-structure-property relationships in PTFE expansion.
- Enabled several new product prototypes such as arterial stent grafts, arterial shunts, or hernia patches by creating PTFE membrane prototypes specifically optimized for each application.
- Reduced operating costs on several manufacturing processes by up to 70% by using both historical data and my experimental data to redesign and optimize the processes. Implemented all process changes in an FDA-regulated environment while simultaneously overseeing day-to-day manufacturing of several products.

Undergraduate Researcher — University of Delaware, Newark DE
Modeling and control of glycosylation — *March 2010—May 2011*

- Constructed both deterministic and stochastic-Monte-Carlo microkinetic models to predict the glycosylation/product quality of monoclonal antibodies.
- Executed sensitivity analyses on models to assess the feasibility of glycosylation control.
- Documented work via senior thesis.

Intern — W.L. Gore & Associates, Elkton MD
Fuel cell process development — *May 2010—February 2011*

- Developed a new, aqueous process for depositing electrodes onto proton exchange membranes for use in fuel cells.
- Developed scaling relationships between a lab-scale, Meyer-bar coating process and a pilot-scale coating process to reduce development times between new lab-scale and pilot-scale processes.

Intern — W.L. Gore & Associates, Elkton MD
Steam sterilization — *May 2009—August 2009*

- Designed, purchased, and validated steam sterilization equipment in an FDA-regulated quality system.

Lab Assistant — Institute of Energy Conversion, Newark DE
PVC image analysis — *September 2007–May 2009*

- Developed software to quantify the size and distribution of grain boundaries on lab-scale copper-indium-galium-selenide photovoltaic cells. Used the software to establish a testing protocol, enabling automated and consistent characterization of photovoltaic cells.
- Assisted with various lab maintenance duties.

TEACHING & MENTORING EXPERIENCE

Group Mentor — Carnegie Mellon University, Pittsburgh PA
Chemical Engineering — *January 2016–January 2021*

- As the first student of a new assistant professor, I was involved in the training and mentoring of every new member in the research group. This includes training three other PhD students in programming, machine learning, and project management skills, along with several undergraduate and master's students.

Teaching Assistant — Carnegie Mellon University, Pittsburgh PA
Chemical Engineering — *August 2016–December 2017*

· Teaching assistant for freshman lab courses, senior lab courses, and master's kinetics classes.

New-graduate Engineer Mentor W.L. Gore & Associates, Elkton MD
Core Technology Division *August 2013–July 2016*

· Mentored several new-graduate engineers in statistical process controls, design of experiments, best manufacturing practices, and best validation practices. Ultimately helped train four engineers to become independent and productive.

Volunteer Tutor & Lego League Coach Boys & Girls Club, Newark DE

· Coached classes of elementary school children to build Lego machines for competition.
· Tutored elementary school children in math.

Tutor University of Delaware, Newark DE
Chemistry *September 2009–May 2010*

· Tutored freshman level chemistry courses.

PUBLICATIONS

Ulissi, Z. W. *et al.* Computational Catalysis, Chapter 6: Practical application of machine learning in catalysis (2024).

Mule, A. S. *et al.* Advancing insights into electrochemical pre-treatments of supported nanoparticle electrocatalysts by combining a design of experiments strategy with in situ characterization. en. *Adv. Energy Mater.* (Aug. 2024).

Chanussot, L. *et al.* Open catalyst 2020 (OC20) dataset and community challenges. en. *ACS Catal.* **11,** 6059–6072 (May 2021).

Tran, K. *et al.* Computational catalyst discovery : Active classification through myopic multiscale sampling. *The Journal of Chemical Physics* **154,** 1–12. `https://aip.scitation.org/doi/pdf/10.1063/5.0044989` (2021).

Zitnick, C. L. *et al.* An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage. arXiv: `2010.09435`. `http://arxiv.org/abs/2010.09435` (2020).

Tran, K. *et al.* Methods for comparing uncertainty quantifications for material property predictions. *Machine Learning: Science and Technology* (2020).

Back, S., Tran, K. & Ulissi, Z. W. Discovery of Acid-Stable Oxygen Evolution Catalysts: High-Throughput Computational Screening of Equimolar Bimetallic Oxides. *ACS Applied Materials & Interfaces.* ISSN: 1944-8244 (2020).

Back, S., Na, J., Tran, K. & Ulissi, Z. W. In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation. en. *Phys. Chem. Chem. Phys.* **22,** 19454–19458 (Sept. 2020).

Lopato, E. M. *et al.* Parallelized Screening of Characterized and DFT-Modelled Bimetallic Colloidal Co-Catalysts for Photocatalytic Hydrogen Evolution. *ACS Catalysis,* 4244–4252 (2020).

Zhong, M. *et al.* Accelerated discovery of CO2 electrocatalysts using active machine learning. *Nature* **581,** 178–183. ISSN: 0028-0836. `http://www.nature.com/articles/s41586-020-2242-8` (2020).

Hanselman, C., Zhong, W., Tran, K., Ulissi, Z. W. & Gounaris, C. Optimization-Based Design of Active and Stable Nanostructured Surfaces. *Journal of Physical Chemistry C* (2019).

Back, S., Tran, K. & Ulissi, Z. W. Toward a Design of Active Oxygen Evolution Catalysts: Insights from Automated Density Functional Theory Calculations and Machine Learning. *ACS Catalysis,* 7651–7659. ISSN: 2155-5435. `http://pubs.acs.org/doi/10.1021/acscatal.9b02416` (2019).

Aini, P., Zhong, W., Tran, K., Back, S. & Ulissi, Z. W. Towards Predicting Intermetallics Surface Properties with High-Throughput DFT and Convolutional Neural Networks. *Journal of Chemical Information and Modeling* **59,** 4742–4749 (2019).

Back, S. *et al.* Convolutional Neural Network of Atomic Surface Structures To Predict Binding Energies for High-Throughput Screening of Catalysts. *The Journal of Physical Chemistry Letters* **10,** 4401–4408. ISSN: 1948-7185 (2019).

Tran, K., Aini, P., Back, S. & Ulissi, Z. W. Dynamic Workflows for Routine Materials Discovery in Surface Science. *Journal of Chemical Information and Modeling* **58,** 2392–2400 (2018).

Tran, K. & Ulissi, Z. W. Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution. *Nature Catalysis* **1,** 696–703 (2018).

St Amand, M. M., Tran, K., Radhakrishnan, D., Robinson, A. S. & Ogunnaike, B. A. Controllability analysis of protein glycosylation in Cho cells. *PLoS ONE* **9** (2014).

TALKS/PRESENTATIONS

K. Tran, Z. Ulissi, "Methods for Computational Catalyst Discovery", *Chegsa Symposium*, Pittsburgh, PA (October 2020).

K. Tran, Z. Ulissi, "Active Optimization of Sustainable Energy and Chemistries" (**invited**), *Data Science Institute, Lawrence Livermore National Lab*, Livermore, CA (June 2019).

K. Tran, Z. Ulissi, "DFT Screening of Electrocatalysts Using Active Optimization", *North American Catalysis Society Meeting*, Chicago, IL (June 2019).

K. Tran, "Active Learning for Materials Design" (**invited**), *This Week in Machine Learning & AI*, https://twimlai.com (March 2019).

K. Tran, Z. Ulissi, "Methods to Exploit Large Datasets in Catalysis", *AIChE Annual Meeting*, Pittsburgh, PA (November 2018).

K. Tran, Z. Ulissi, "Active Learning across Intermetallics Guides Discovery of Electrocatalysts for Carbon Dioxide Reduction and Hydrogen Evolution", *AIChE Annual Meeting*, Pittsburgh, PA (October 2018).

C.L. Hanselman, W. Zhong, K. Tran, Z. Ulissi, C.E. Gounaris, "Design of Optimal Metallic Surface Reconstruction for Heterogeneous Catalysis" (poster), *AIChE Annual Meeting*, Pittsburgh, PA (October 2018).

W. Zhong, C.L. Hanselman, K. Tran, Z. Ulissi, C.E. Gounaris, "Prediction of Surface Energies for Complex Pt Structures from Coordination Number and Generalized Coordination Number" (poster), *AIChE Annual Meeting*, Pittsburgh, PA (October 2018).

K. Tran, Z. Ulissi, "Improving sustainable energy storage with active machine learning" (poster), *Machine Learning in Science and Engineering*, Pittsburgh, PA (June 2018).

K. Tran, Z. Ulissi, "Discovering catalysts for CO_2 reduction using an automated DFT framework" (poster), *Surrogate Models and Coarsening Techniques: IPAM Workshop III*, Los Angeles, CA (November 2017).

HONORS & AWARDS

Ken Meyer Award, Carnegie Mellon University	*2021*
Chegsa Symposium Award for oral presentation, Carnegie Mellon University	*2020*
Kokes Award, North American Catalysis Society	*2019*
Science Graduate Student Research (SCGSR) award (*declined*), Department of Energy	*2019*
Bushnell Fellowship, Carnegie Mellon University	*2019*
Honors Degree with Distinction, University of Delaware	*2011*
Dean's list, University of Delaware	*2007–2011*
Hess Corporation Award	*2010*
Engineering Alumni Association Award, University of Delaware	*2009*
General Honors Award, University of Delaware	*2009*

PROFESSIONAL MEMBERSHIPS

President, UD Student Chapter of the American Institute of Chemical Engineers (AIChE)	*2010–2011*
Treasurer, UD Student Chapter of AIChE	*2008–2010*