

# KEVIN TRAN

Curriculum Vitae ♦ Updated on 27 April 2021

Schrödinger ♦ Materials Science Division ♦ New York, NY 10036

## EDUCATION

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<b>Carnegie Mellon University</b> PhD in Chemical Engineering	<i>2016–2021</i>
<b>University of Delaware</b> Bachelor's of Science in Chemical Engineering, Minor in Philosophy	<i>2007–2011</i>

## EMPLOYMENT HISTORY

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

## WORK & RESEARCH EXPERIENCE

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<b>Senior Scientist</b> <i>Materials Science Development</i>	Schrödinger, New York NY <i>April 2021–present</i>
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- I develop and maintain software that performs, manages, and analyzes molecular dynamics and density functional theory simulations. We use these simulations to help scientists discover and optimize new materials for several applications.

<b>Graduate Research Assistant</b> <i>Chemical Engineering</i>	Carnegie Mellon University, Pittsburgh PA <i>August 2016–January 2021</i>
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- 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 machine learning optimization 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 process to reduce development times between new lab-scale and pilot-scale processes.

**Intern***Steam sterilization*

W.L. Gore &amp; Associates, Elkton MD

*May 2009—August 2009*

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

**Lab Assistant***PVC image analysis*

Institute of Energy Conversion, Newark DE

*September 2007–May 2009*

- Developed image analysis methods to characterize and quantify grain boundaries of copper-indium-gallium-selenide photovoltaic cells, thereby establishing a new quantitative testing protocol for new photovoltaic samples.
- Assisted with various lab maintenance duties.

**TEACHING & MENTORING EXPERIENCE**

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**Group Mentor***Chemical Engineering*

Carnegie Mellon University, Pittsburgh PA

*January 2016–Present*

- As the first student of a new assistant professor, I was involved in the training and mentoring of almost every member in our 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***Chemical Engineering*

Carnegie Mellon University, Pittsburgh PA

*August 2016–December 2017*

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

**New-graduate Engineer Mentor***Core Technology Division*

W.L. Gore &amp; Associates, Elkton MD

*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 &amp; Girls Club, Newark DE

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

**Tutor***Chemistry*

University of Delaware, Newark DE

*September 2009–May 2010*

- Tutored freshman level chemistry courses.

**PUBLICATIONS**

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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).

Chanussot, L. *et al.* The Open Catalyst 2020 (OC20) Dataset and Community Challenges. **2020**. arXiv: 2010.09990. <http://arxiv.org/abs/2010.09990> (2020).

- 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).
- 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 CO<sub>2</sub> 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 CO<sub>2</sub> reduction and H<sub>2</sub> 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

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- 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<sub>2</sub> reduction using an automated DFT framework” (poster), *Surrogate Models and Coarsening Techniques: IPAM Workshop III*, Los Angeles, CA (November 2017).

## HONORS & AWARDS

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Chegsa Symposium Award for oral presentation, Carnegie Mellon University	2020
Kokes Award, North American Catalysis Society	2019
Science Graduate Student Research (SCGSR) award ( <i>declined</i> ), 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

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