Zachary W. Ulissi

Research Scientist · Meta Fundamental AI Research

250 Howard Street, San Francisco CA 94105

zulissi@gmail.com | https://zulissi.github.io | zulissi | zulissi | Zachary W. Ulissi

Positions

Meta Fundamental AI Research (FAIR) Research Scientist — *San Francisco, CA (01/2023 - present)*
Carnegie Mellon University Adjunct Prof. of Chem. Eng. — *Pittsburgh, PA (01/2024 - present)*
Carnegie Mellon University Assoc. Prof. (w/o Tenure) of Chem. Eng. and (courtesy) MSE — *Pittsburgh, PA (07/2022 - 12/2023)*
Carnegie Mellon University Asst. Prof. of Chemical Eng. and (courtesy) Mat. Sci. and Eng. — *Pittsburgh, PA (08/2017 - 06/2022)*
Stanford University / SLAC Postdoctoral Fellow, Chemical Engineering — *Stanford, CA (07/2015 - 07/2017)*

Education

Massachusetts Institute of Technology Ph.D. in Chem. Eng.; M. Strano and R. Braatz — *Cambridge, MA (09/2010 - 06/2015)*
Churchill College, University of Cambridge M.A.St. in Applied Math and Theoretical Physics — *Cambridge, UK (09/2009 - 06/2010)*
University of Delaware Honors B.E. in Chemical Engineering, Honors B.S. in Physics — *Newark, Delaware (09/2005 - 05/2009)*

Honors & Awards

2022 **Dean's Early Career Fellow**, Outstanding research accomplishments and potential — *Engineering, CMU*
2021 **G.T. Ladd Research Award**, Outstanding research accomplishments and potential — *Engineering, CMU*
2020 **AIChE 35 under 35**, Members under 35 who have made sig. contributions to the field of Chem. Eng. — *AIChE*
2020-2023 **3M Non-Tenured Faculty Award**, Research support and interaction with 3M — *3M*
2020-2022 **ACS PRF Doctoral New Investigator**, Research support for preliminary project — *ACS PRF*
2019-2023 **Scott Institute for Energy Innovation Fellow**, Logistics/support to promote energy research at CMU — *CMU*
2019 **Scialog Fellow**, Fellowship for the Scialog Conference in Energy Storage — *Scialog Foundation*
2018 **Wimmer Fellow**, Fellowship to improve 06-625 Chemical and Reactive Systems course — *Eberly Center, CMU*
2017 **Team Science Award**, "Materials disc., theory, and charact. of intermetallics for electro. CO2 reduction" — *DOE EFRC Meeting*
2010-2014 **DOE CSGF Fellow**, Four years of support, interaction with DOE computational science community — *DOE*
2009-2010 **NSF GRFP Fellow**, Three years of partial fellowship support — *NSF*

Teaching

UG: Numerical Methods and Machine Learning for Chemical Engineering Z Ulissi — *06-325 (Fall 2022)*
UG: Mathematical Methods of Chemical Engineering Zachary Ulissi — *06-262 (Spring 2019-2022)*
MS: Chemical and Reactive Systems Zachary Ulissi — *06-625 (Fall 2017-2020)*

Research Group (CMU)

Alumni Nicholas Tiwari (PhD, Changed Advisor), Kirby Broderick (PhD, Changed Advisor), Unnatti Sharma (PhD, Changed Advisor), Joseph Musielewicz (PhD, Changed Advisor), Adeesh Kolluru (PhD, Changed Advisor), Xiaoxiao (Lory) Wang (PhD, Changed Advisor), Brook Wander (PhD, Changed Advisor), Rohan (Yuri) Sanspeur(PhD, Changed Advisor), Hilda Mera (MS 2023), Ethan Sunshine (PhD, Changed Advisor), Janghoon Ock (PhD, Changed Advisor), Javier Heras Domingo (Post-doc 2023, ICIQ), Tian Tian (Post-doc 2023, Faculty U.Alberta), Richard Tran (Post-doc 2023, Post-doc U.Houston), Kyung-Eun You (Post-doc 2023, Post-doc UPitt), Aaron Garrison (UG 2023, PhD MIT), Anna Maria Ferrante (UG 2024), Logan Meritz (UG 2025), Muhammed Shuaibi (PhD 2022, Meta FAIR), Kevin Tran (PhD 2021, Schrodinger), Amish Chovatiya (MS 2019, Intermolecular, now PhD Notre Dame), Katsuyuki Tomita (MS 2019, Nippon Steel), Nianhan (Kaylee) Tian (UG/MS 2020, PhD G.Tech), Seoin Back (PD, faculty at Sogang University), Zong Qian Yu (MS 2018), Wen Zhong (MS 2018, consulting), Hyukjae Kwark (BS 2020), Shiv Rekhi (MS 2019, co-advised w/ Kathryn Whitehead, PhD Lehigh), Tanmay Raj (MS 2019, Cargill), Qingyang Zhang (MS 2019, RA with Venkat Viswanathan), Sudheesh Ethirajan (MS 2020, PhD UC Davis), Jingxuan Li (MS 2020), Arundhati Madabhushi (MS 2020, Consultant at BCG), Matthew Adams (MS 2020, EPA), Rui Qi Chen (UG 2021, PhD GTech), Ketong Chen (UG 2022), Megan McGraw (UG 2022), Jasmine Fahrenkrug (UG, 2022), Saurabh Pattabiraman (MS 2020, PhD UC Davis), Ziheng (Daniel) Liu (UG 2021), Aini Palizhati (PhD 2022, Boston Consulting Group), Junwoong Yoon (PhD 2022, Meta), Rajesh Raju (Post-Doc, MS at MILA)

Invited Talks and Seminars

ECOMATES School on in-silico Methods for Catalyst Design Zachary Ulissi — *Dublin, IE (Remote) (3/2025)*
University of Chicago Department of Geophysical Sciences Seminar Zachary Ulissi — *Chicago, Il (2/2025)*
Learning on Graphs (LoG) Conference Keynote Zachary Ulissi — *Remote (11/2024)*
Block AI Keynote on AI for Science Zachary Ulissi — *Oakland, CA (11/2025)*
Northwestern University Research Seminar Zachary Ulissi — *Evanston, Il (10/2024)*
AIMED Workshop on Heterogeneous Catalysis Zachary Ulissi — *Chicago, Il (10/2024)*
UChicago Schmidt Science Fellows AI+Science Summer School Zachary Ulissi — *Chicago, Il (7/2024)*
Nobel Turing Challenge Initiative Keynote Zachary Ulissi — *Singapore, SG (7/2024)*
NTU University Research Seminar Zachary Ulissi — *Nanyang, SG (7/2024)*
Shell.ai Aryabhata Seminar Series Zachary Ulissi — *US (Remote) (6/2024)*
Simons Institute AI=Science Workshop Zachary Ulissi — *Berkeley, CA (6/2024)*
Stahl Forum Zachary Ulissi — *Minneapolis, MN (4/2024)*
Aionics Industrial Seminar Zachary Ulissi — *US (Remote) (4/2024)*
TACO (Taming Complexity Together) PhD Retreat Zachary Ulissi — *Austria (Remote) (2/2024)*
NYU/Simons Center for Comp. Phys. Chem. Zachary Ulissi — *New York, NY (11/2023)*
Northeastern University Mechanical and Industrial Eng. Zachary Ulissi — *Boston, MA (11/2023)*
LBL Advanced Light Source Zachary Ulissi — *Berkeley (CA) (09/2023)*
Climate Change AI Web Seminar Zachary Ulissi — *US (Remote) (09/2023)*
Foundations of Process Analytics and Machine Learning (FOPAM) Zachary Ulissi — *Davis, CA (08/2023)*
ACS Symposium on Data Science in Catalysis: Catalysis Informatics Zachary Ulissi — *San Francisco, CA (08/2023)*
ACS Symposium on Data Science in Catalysis Zachary Ulissi — *San Francisco, CA (08/2023)*
ACS Symposium in Honor of AJ Medford Zachary Ulissi — *San Francisco, CA (08/2023)*
Telluride Science Zachary Ulissi — *Telluride, CO (07/2023)*
Dow Chemical Zachary Ulissi — *US (Remote) (07/2023)*
ICLR ML4Materials Workshop Zachary Ulissi — *US (Remote) (05/2023)*
Georgia Tech Chemical and Biomolecular Engineering Zachary Ulissi — *Atlanta, GA (4/2023)*
Center for Environmentally Beneficial Catalysis Zachary Ulissi — *US (remote) (3/2023)*
Great Plains Catalysis Society Zachary Ulissi — *US (remote) (11/2022)*
Great Plains Catalysis Society Zachary Ulissi — *US (remote) (11/2022)*
Toyota Research Institute Zachary Ulissi — *Los Altos, CA (remote) (11/2022)*
Catalyst Modeling Symposium Zachary Ulissi — *Rungstedgaard, DK (9/2022)*
ACS Fall National Meeting Zachary Ulissi — *Chicago, IL (8/2022)*
NIST Artificial Intelligence for Materials Science (AIMS) Symposium Zachary Ulissi — *Gaithersburg, MD (remote) (7/2022)*
Nano Korea Zachary Ulissi — *Korea (remote) (7/2022)*
Machine Learning for Materials (ML4M) Zachary Ulissi — *Trieste, Italy (5/2022)*
NanoGe Conference Zachary Ulissi — *Spain (remote) (3/2022)*
Monash University Zachary Ulissi — *Melbourne, Australia (remote) (3/2022)*
Heraeus Workshop Zachary Ulissi — *Germany (remote) (1/2022)*
Technical University Delft Zachary Ulissi — *Delft, NL (remote) (11/2021)*
3M Young Faculty Symposium Zachary Ulissi — *St Paul, MN (remote) (11/2021)*
German Young Professional Engineers Seminar Series (NaWuReT) Zachary Ulissi — *Germany (remote) (10/2021)*
ACS Fall Meeting Symposium Keynote Zachary Ulissi — *Atlanta, GA (8/2021)*
Materials Project Seminar Series Zachary Ulissi — *Berkeley, CA (remote) (8/2021)*
Statistical Thermodynamics and Molecular Simulation (STMS) Series Zachary Ulissi — *Remote (6/2021)*
Telluride Workshop on Computational Materials Chemistry Zachary Ulissi — *Telluride, CO (6/2021)*
Colloid and Surface science Symposium Zachary Ulissi — *State College, PA (remote) (6/2021)*
International Workshop on Computer-Aided Materials Discovery Zachary Ulissi — *Korea (remote) (6/2021)*
OPTIMADE workshop Zachary Ulissi — *Louvain, Belgium (remote) (6/2021)*
DOE NERSC Data Seminar Zachary Ulissi — *Berkeley, CA (remote) (4/2021)*
North Carolina State University Dept of Chem. and Biom. Eng. Zachary Ulissi — *Raleigh, NC (remote) (4/2021)*
Penn Institute for Computational Science Zachary Ulissi — *Philadelphia, PA (remote) (3/2021)*
3M Young Faculty Symposium Zachary Ulissi — *St Paul, MN (remote) (2/2021)*
Matminer Singapore Seminar Series Zachary Ulissi — *Singapore (remote) (12/2020)*
Fritz-Haber Institute Theory Seminar Zachary Ulissi — *Berlin, GE (remote) (12/2020)*
DTRA Annual Review External Speaker Zachary Ulissi — *Aberdeen, MD (remote) (11/2020)*
3M Zachary Ulissi — *St Paul, MN (remote) (11/2020)*
Dow Zachary Ulissi — *Midlands, MI (remote) (11/2020)*

EcoCAT Symposium Zachary Ulissi *Barcelona, Spain (remote)* (*11/2020*)
NERSC Deep Learning for Science Lecture Zachary Ulissi *LBL, Berkeley, CA (remote)* (*10/2020*)
RAPID ML in Sci/Eng. Seminar Zachary Ulissi *Newark, DE (remote)* (*7/2020*)
DTU Catalysis Theory Seminar Zachary Ulissi *Lyngby, DK (remote)* (*6/2020*)
Lyondell Bassell Zachary Ulissi *Houston, TX (remote)* (*5/2020*)
Citrine Informatics Zachary Ulissi *Redwood City, CA* (*3/2020*)
DOE NERSC Data Seminar Zachary Ulissi *LBL, Berkeley, CA* (*3/2020*)
Symposium on AI in Chemical Engineering Zachary Ulissi *ETH Zürich, Switzerland* (*2/2020*)
MRS Fall Meeting Zachary Ulissi *Boston, MA* (*12/2019*)
Chemistry Meets AI Symposium Zachary Ulissi *KAIST, Daejeon, Korea* (*11/2019*)
International Conference on Molecular Simulation Zachary Ulissi *Jeju Island, Korea* (*11/2019*)
University of Delaware Department of Physics Zachary Ulissi *Newark, DE* (*10/2019*)
University of Washington Department of Chemical Engineering Zachary Ulissi *Seattle, WA* (*10/2019*)
NIST Artificial Intelligence for Materials Science (AIMS) Workshop Zachary Ulissi *Gaithersburg, MD* (*08/2019*)
Lehigh University Inst for Data, Intelligent Systems, and Comp Z Ulissi *Bethlehem, PA* (*05/2019*)
Keynote for Virginia Tech Chem. Eng. Graduate Student Symposium Zachary Ulissi *Blacksburg, VA* (*04/2019*)
ExxonMobil Research and Development Zachary Ulissi *Annandale, PA* (*04/2019*)
COMET NSF IGERT Training Center Seminar Zachary Ulissi *State College, PA* (*11/2018*)
Pittsburgh Cleveland Catalysis Society Annual Symposium Zachary Ulissi *Pittsburgh, PA* (*6/2018*)
Workshop: Accelerating the Dev. of Energy Mat. and Novel Structural Mat. Z Ulissi *Toronto, CA* (*5/2018*)
Materials Science Division, Lawrence Livermore National Laboratory Zachary Ulissi *Livermore, CA* (*5/2018*)
ACS Spring Meeting Zachary Ulissi *New Orleans, LA* (*3/2018*)
University of Auckland Department of Chem. Engineering Zachary Ulissi *Auckland, NZ* (*2/2018*)
University of Toronto Department of Electrical Engineering Zachary Ulissi *Toronto, CA* (*11/2017*)
Institute for Pure and Applied Mathematics Workshop Series Zachary Ulissi *Los Angeles, CA* (*10/2017*)
Machine Learning for Energy Materials CIFAR Workshop Zachary Ulissi *Toronto, CA* (*5/2017*)

Publications, Pre-Prints, Conf. Papers, Chapters, and Tech. Reports

[**83**] **Pourbaix Machine Learning Framework Identifies Acidic Water Oxidation Catalysts Exhibiting Suppressed Ruthenium Dissolution**

J. Abed, J. Heras-Domingo, R. Y. Sanspeur, M. Luo, W. Alnoush, D. M. Meira, H. Wang, J. Wang, J. Zhou, D. Zhou ***Journal of the American Chemical Society***. 2024

[**82**] **Open Catalyst Experiments 2024 (OCx24): Bridging Experiments and Computational Models**

J. Abed, J. Kim, M. Shuaibi, B. Wander, B. Duijf, S. Mahesh, H. Lee, V. Gharakhanyan, S. Hoogland, E. Irtem, J. Lan, N. Schouten, A. U. Vijayakumar, J. Hattrick-Simpers, J. R. Kitchin, Z. W. Ulissi, A. Vugt, E. H. Sargent, D. Sinton, C. L. Zitnick . 2024

[**81**] **Open materials 2024 (omat24) inorganic materials dataset and models**

L. Barroso-Luque, M. Shuaibi, X. Fu, B. M. Wood, M. Dzamba, M. Gao, A. Rizvi, C. L. Zitnick, Z. W. Ulissi ***arXiv preprint arXiv:2410.12771***. 2024

[**80**] **Adapting OC20-Trained EquiformerV2 Models for High-Entropy Materials**

C. M. Clausen, J. Rossmeisl, Z. W. Ulissi ***The Journal of Physical Chemistry C*** pp. 11190–11195, 2024

[**79**] **Fine-Tuned Language Models Generate Stable Inorganic Materials as Text**

N. Gruver, A. Sriram, A. Madotto, A. Wilson, C. L. Zitnick, Z. Ulissi ***ICLR***. 2024

[**78**] **Enumeration of surface site nuclearity and shape in a database of intermetallic low-index surface facets**

U. Sharma, A. Nguyen, J. R. Kitchin, Z. W. Ulissi, M. J. Janik ***Journal of Catalysis*** p. 115795, 2024

[**77**] **From Molecules to Materials: Pre-training Large Generalizable Models for Atomic Property Prediction**

N. Shoghi, A. Kolluru, J. R. Kitchin, Z. W. Ulissi, C. L. Zitnick, B. M. Wood ***ICLR***. 2024

[**76**] **The Open DAC 2023 Dataset and Challenges for Sorbent Discovery in Direct Air Capture**

A. Sriram, S. Choi, X. Yu, L. M. Brabson, A. Das, Z. Ulissi, M. Uyttendaele, A. J. Medford, D. S. Sholl ***ACS Central Science*** pp. 923–941, 2024

[**75**] **chap. Chapter 6: Practical Application of Machine Learning in Catalysis** Z. W. Ulissi, K. Tran, J. Yoon, M. Shuaibi, M. Liu, N. Zhan, K. Broderick, J. R. Kitchin "Computational Catalysis", 2024

[**74**] **CatTSunami: Accelerating Transition State Energy Calculations with Pre-trained Graph Neural Networks**

B. Wander, M. Shuaibi, J. R. Kitchin, Z. W. Ulissi, C. L. Zitnick ***arXiv preprint arXiv:2405.02078***. 2024

[**73**] **Generalization of graph-based active learning relaxation strategies across materials**

X. Wang, J. Musielewicz, R. Tran, S. K. Ethirajan, X. Fu, H. Mera, J. R. Kitchin, R. C. Kurchin, Z. W. Ulissi ***Machine Learning: Science and Technology*** p. 025018, 2024

[72] **Applying Large Graph Neural Networks to Predict Transition Metal Complex Energies Using the tmQM_wB97MV Data Set**

A. G. Garrison, J. Heras-Domingo, J. R. Kitchin, G. Passos Gomes, Z. W. Ulissi, S. M. Blau ***Journal of Chemical Information and Modeling***. 2023

[71] **AdsorbML: a leap in efficiency for adsorption energy calculations using generalizable machine learning potentials**

J. Lan, A. Palizhati, M. Shuaibi, B. M. Wood, B. Wander, A. Das, M. Uyttendaele, C. L. Zitnick, Z. W. Ulissi ***npj Computational Materials*** p. 172, 2023

[70] **Beyond independent error assumptions in large GNN atomistic models**

J. Ock, T. Tian, J. Kitchin, Z. Ulissi ***The Journal of Chemical Physics***. 2023

[69] **Cluster-MLP: An Active Learning Genetic Algorithm Framework for Accelerated Discovery of Global Minimum Configurations of Pure and Alloyed Nanoclusters**

R. K. Raju, S. Sivakumar, X. Wang, Z. W. Ulissi ***Journal of Chemical Information and Modeling***. 2023

[68] **WhereWulff: A Semiautonomous Workflow for Systematic Catalyst Surface Reactivity under Reaction Conditions**

R. Y. Sanspeur, J. Heras-Domingo, J. R. Kitchin, Z. Ulissi ***Journal of Chemical Information and Modeling*** pp. 2427–2437, 2023

[67] **AmpTorch: A Python package for scalable fingerprint-based neural network training on multi-element systems with integrated uncertainty quantification**

M. Shuaibi, Y. Hu, X. Lei, B. M. Comer, M. Adams, J. Paras, R. Q. Chen, E. Musa, J. Musielewicz, A. A. Peterson ***Journal of Open Source Software*** p. 5035, 2023

[66] **Chemical Properties from Graph Neural Network-Predicted Electron Densities**

E. M. Sunshine, M. Shuaibi, Z. W. Ulissi, J. R. Kitchin ***The Journal of Physical Chemistry C*** pp. 23459–23466, 2023

[65] **The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysts**

R. Tran, J. Lan, M. Shuaibi, B. M. Wood, S. Goyal, A. Das, J. Heras-Domingo, A. Kolluru, A. Rizvi, N. Shoghi, A. Sriram, F. Therrien, J. Abed, O. Voznyy, E. H. Sargent, Z. Ulissi, C. L. Zitnick ***ACS Catalysis*** pp. 3066–3084, 2023

[64] **Identifying limitations in screening high-throughput photocatalytic bimetallic nanoparticles with machine-learned hydrogen adsorptions**

K. Broderick, E. Lopato, B. Wander, S. Bernhard, J. Kitchin, Z. Ulissi ***Applied Catalysis B: Environmental*** p. 121959, 2023

[63] **How Do Graph Networks Generalize to Large and Diverse Molecular Systems?**

J. Gasteiger, M. Shuaibi, A. Sriram, S. Günnemann, Z. Ulissi, C. L. Zitnick, A. Das ***arXiv preprint arXiv:2204.02782***. 2022

[62] **Transfer learning using attentions across atomic systems with graph neural networks (TAAG)**

A. Kolluru, N. Shoghi, M. Shuaibi, S. Goyal, A. Das, C. L. Zitnick, Z. Ulissi ***The Journal of Chemical Physics*** p. 184702, 2022

[61] **Detailed Microkinetics for the Oxidation of Exhaust Gas Emissions through Automated Mechanism Generation**

B. Kreitz, P. Lott, J. Bae, K. Blöndal, S. Angeli, Z. W. Ulissi, F. Studt, C. F. Goldsmith, O. Deutschmann ***ACS Catalysis*** pp. 11137–11151, 2022

[60] **Predicting Oxidation Behavior of Multi-Principal Element Alloys by Machine Learning Methods**

J. A. Loli, A. R. Chovatiya, Y. He, Z. W. Ulissi, M. P. Boer, B. A. Webler ***Oxidation of Metals*** pp. 429–450, 2022

[59] **Heterogeneous Catalysis in Grammar School**

J. T. Margraf, Z. W. Ulissi, Y. Jung, K. Reuter ***The Journal of Physical Chemistry C*** pp. 2931–2936, 2022

[58] **Site Geometry as a Descriptor for Catalyst Selectivity in Intermetallics**

U. Sharma, A. Nguyen, M. J. Janik, Z. Ulissi ***Preprint available at SSRN 4145497***. 2022

[57] **Screening of bimetallic electrocatalysts for water purification with machine learning**

R. Tran, D. Wang, R. Kingsbury, A. Palizhati, K. A. Persson, A. Jain, Z. W. Ulissi ***The Journal of Chemical Physics*** p. 074102, 2022

[56] **The Open Catalyst Challenge 2021: Competition Report**

A. Das, M. Shuaibi, A. Palizhati, S. Goyal, A. Grover, A. Kolluru, J. Lan, A. Rizvi, A. Sriram, B. Wood, D. Parikh, Z. Ulissi, C. L. Zitnick, G. Ke, S. Zheng, Y. Shi, D. He, T.-Y. Liu, C. Ying, J. You, Y. He, R. Grigoriev, R. Lukin, A. Yarullin, M. Faleev pp. 29–40, 2022

[55] **Robust and scalable uncertainty estimation with conformal prediction for machine-learned interatomic potentials**

Y. Hu, J. Musielewicz, Z. W. Ulissi, A. J. Medford ***Machine Learning: Science and Technology*** p. 045028, 2022

[54] **Spherical Channels for Modeling Atomic Interactions**

C. L. Zitnick, A. Das, A. Kolluru, J. Lan, M. Shuaibi, A. Sriram, Z. Ulissi, B. Wood ***NeurIPS***. 2022

[53] **FINETUNA: Fine-tuning Accelerated Molecular Simulations**

J. Musielewicz, X. Wang, T. Tian, Z. W. Ulissi ***Machine Learning: Science and Technology***. 2022

[52] **Catlas: an automated framework for catalyst discovery demonstrated for direct syngas conversion**

B. Wander, K. Broderick, Z. W. Ulissi ***Catal. Sci. Technol.*** pp. -, 2022

The Open Catalyst Challenge 2021: Competition Report.

A. Das, M. Shuaibi, A. Palizhati, S. Goyal, A. Grover, A. Kolluru, J. Lan, A. Rizvi, A. Sriram, B. M. Wood

NeurIPS (Competition and Demos), 2021

[**50**]**Elimination of Multidrug-Resistant Bacteria by Transition Metal Dichalcogenides Encapsulated by Synthetic Single-Stranded DNA**

A. Debnath, S. Saha, D. O. Li, X. S. Chu, Z. W. Ulissi, A. A. Green, Q. H. Wang ***ACS Applied Materials & Interfaces*** pp. 8082–8094, 2021

[**49**]**Rotation Invariant Graph Neural Networks using Spin Convolutions**

M. Shuaibi, A. Kolluru, A. Das, A. Grover, A. Sriram, Z. Ulissi, C. L. Zitnick ***arXiv preprint arXiv:2106.09575***. 2021

[**48**]**Computational catalyst discovery: Active classification through myopic multiscale sampling**

K. Tran, W. Neiswanger, K. Broderick, E. Xing, J. Schneider, Z. W. Ulissi ***The Journal of Chemical Physics*** p. 124118, 2021

[**47**]**Deep reinforcement learning for predicting kinetic pathways to surface reconstruction in a ternary alloy**

J. Yoon, Z. Cao, R. K. Raju, Y. Wang, R. Burnley, A. J. Gellman, A. B. Farimani, Z. W. Ulissi ***Machine Learning: Science and Technology*** p. 045018, 2021

[**46**]**Open Catalyst 2020 (OC20) Dataset and Community Challenges**

L. Chanussot, A. Das, S. Goyal, T. Lavril, M. Shuaibi, M. Riviere, K. Tran, J. Heras-Domingo, C. Ho, W. Hu, A. Palizhati, A. Sriram, B. Wood, J. Yoon, D. Parikh, C. L. Zitnick, Z. Ulissi ***ACS Catalysis*** pp. 6059–6072, 2021

[**45**]**Efficient Discovery of Active, Selective, and Stable Catalysts for Electrochemical H_2O_2 Synthesis through Active Motif Screening**

S. Back, J. Na, Z. W. Ulissi ***ACS Catalysis*** pp. 2483–2491, 2021

[**44**]**Differentiable Optimization for the Prediction of Ground State Structures (DOGSS)**

J. Yoon, Z. W. Ulissi ***Physical Review Letters*** p. 173001, 2020

[**43**]**An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage**

C. L. Zitnick, L. Chanussot, A. Das, S. Goyal, J. Heras-Domingo, C. Ho, W. Hu, T. Lavril, A. Palizhati, M. Riviere ***arXiv preprint arXiv:2010.09435***. 2020

[**42**]**Enabling robust offline active learning for machine learning potentials using simple physics-based priors**

M. Shuaibi, S. Sivakumar, R. Q. Chen, Z. W. Ulissi ***Machine Learning: Science and Technology***. 2020

[**41**]**In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation**

S. Back, J. Na, K. Tran, Z. W. Ulissi ***Phys. Chem. Chem. Phys.*** pp. 19454–19458, 2020

[**40**]**Discovery of Acid-Stable Oxygen Evolution Catalysts: High-throughput Computational Screening of Equimolar Bimetallic Oxides**

S. Back, K. Tran, Z. W. Ulissi ***ACS Applied Materials & Interfaces*** pp. 38256–38265, 2020

[**39**]**Computational Notebooks in Chemical Engineering Curricula**

J. Verrett, F. Boukouvala, A. Dowling, Z. Ulissi, V. Zavala ***Chemical Engineering Education*** pp. 143–150, 2020

[**38**]**Methods for comparing uncertainty quantifications for material property predictions**

K. Tran, W. Neiswanger, J. Yoon, Q. Zhang, E. Xing, Z. W. Ulissi ***Machine Learning: Science and Technology*** p. 025006, 2020

[**37**]**Accelerated discovery of CO2 electrocatalysts using active machine learning**

M. Zhong, K. Tran, Y. Min, C. Wang, Z. Wang, C.-T. Dinh, P. De Luna, Z. Yu, A. S. Rasouli, P. Brodersen, S. Sun, O. Voznyy, C.-S. Tan, M. Askerka, F. Che, M. Liu, A. Seifitokaldani, Y. Pang, S.-C. Lo, A. Ip, Z. Ulissi, E. H. Sargent ***Nature*** pp. 178–183, 2020

[**36**]**Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening**

G. H. Gu, J. Noh, S. Kim, S. Back, Z. Ulissi, Y. Jung ***The Journal of Physical Chemistry Letters*** pp. 3185–3191, 2020

[**35**]**Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution**

E. M. Lopato, E. A. Eikey, Z. C. Simon, S. Back, K. Tran, J. Lewis, J. F. Kowalewski, S. Yazdi, J. R. Kitchin, Z. W. Ulissi ***ACS Catalysis*** pp. 4244–4252, 2020

[**34**]**Capturing Structural Transitions in Surfactant Adsorption Isotherms at Solid/Solution Interfaces**

J. Yoon, Z. W. Ulissi ***Langmuir*** pp. 819–826, 2020

[**33**]**Optimization-Based Design of Active and Stable Nanostructured Surfaces**

C. L. Hanselman, W. Zhong, K. Tran, Z. W. Ulissi, C. E. Gounaris ***The Journal of Physical Chemistry C*** pp. 29209–29218, 2019

[**32**]**Towards Predicting Intermetallics Surface Properties with High-Throughput DFT and Convolutional Neural Networks**

A. Palizhati, W. Zhong, K. Tran, S. Back, Z. W. Ulissi ***Journal of Chemical Information and Modeling***. 2019

[**31**]**Toward a Design of Active Oxygen Evolution Catalysts: Insights from Automated Density Functional Theory Calculations and Machine Learning**

S. Back, K. Tran, Z. W. Ulissi ***ACS Catalysis*** pp. 7651–7659, 2019

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External Support (CMU)

Toyota Research Institute PI: Zachary Ulissi, Co-PI: Jeffrey Schneider (*2021-2022*)
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3M Non-Tenured Faculty Award PI: Zachary Ulissi (*2020-2023*)
Lawrence Livermore National Laboratory Subcontract PI: Zachary Ulissi (*2019 - 2021*)
Canadian National Research Council PI: Z Ulissi, Co-PI: I Tamblyn, E Sargent (*2021-2023*)
Army Research Lab PI: Bryan Webler, Co-PI: Maarten de Boer, Zachary Ulissi (*2020-2021*)
Alfred P. Sloan Foundation (Scialog) PI: Anthony (Shoji) Hall, Co-PI: Z. Ulissi, Iryna Zenyuk (*2020-2021*)
DOE ARPA-E PI: Zachary Ulissi, Co-PI: Andrew Gellman, Amir Barati Farimani (*2020-2022*)
Foundation (Wishes to Remain Anonymous) PI: Zachary Ulissi (*2019-2023*)
DOE Advanced Manufacturing Office PI: Anubhav Jain, Co-PI: Zachary Ulissi,Robert Kostecki (*2020 - 2021*)
ACS Petroleum Research Fund PI: Zachary Ulissi (*2020 - 2022*)
DOE BES PI: John Kitchin, Co-PI: Zachary Ulissi, Stefan Bernhard, Jill Millstone (*2019 - 2022*)
DOE BES PI: Michael Janik, Co-PI: Robert Rioux, Zi-Kui Liu, Zachary Ulissi (*2019 - 2022*)
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NSF CBET PI: Andrew Gellman, Co-PI: John Kitchin, Jingguang Chen, Zachary Ulissi (*2019 - 2023*)
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DOE NERSC Cori Supercomputer Allocation PI: Zachary Ulissi *85k CPU, 25k GPU* (*2022*)
DOE NERSC Cori Supercomputer Allocation PI: Zachary Ulissi *28M SU* (*2021*)
DOE NERSC Cori Supercomputer Allocation PI: Zachary Ulissi *28M SU* (*2020*)
DOE NERSC Cori Supercomputer Allocation PI: Zachary Ulissi *16M SU* (*2019*)
DOE NERSC Cori Supercomputer Allocation PI: Zachary Ulissi *13M SU* (*2018*)

Service and Committees (CMU)

CMU Facilities and Space (2019-), Graduate Recruitment (2018-2019), AIChE Undergraduate Adviser (2018-), Chemical Engineering Cube (ChemE Cube) advisor (2020-), Undergraduate Committee (2019-), CIT Cluster Administration (2017-), CIT ad-hoc Research Computing Committee (2020-)

Reviewer Nature Communications, ACS Catalysis, Journal of Physical Chemistry Letters, Journal of Physical Chemistry C, Journal of Vacuum Science and Technology, among many others

Symposia AIChE Annual Meeting (2018-present), MRS Fall Meeting (2019), CMU/GT Machine Learning in Science in Engineering (2018), ACS Spring Meeting (2018)