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 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

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, and Technical Reports

[75] **Multi-Descriptor Design of Ruthenium Catalysts for Durable Acidic Water Oxidation**

J. Abed, J. Heras-Domingo, M. Luo, R. Sanspeur, W. Alnoush, D. Meira, H.-T. Wang, J. Wang, J. Zhou, D. Zhou, K. Fatih, D. Higgins, Z. Ulissi, E. Sargent ***Under Review***. 2023

[74] **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

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

N. Gruver, A. Sriram, A. Madotto, A. Wilson, C. L. Zitnick, Z. Ulissi ***AI for Accelerated Materials Design-NeurIPS 2023 Workshop***. 2023

[72] **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

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

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

[70] **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

[69] **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

[68] **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 ***arXiv preprint arXiv:2310.16802***. 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] **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 ***arXiv preprint arXiv:2311.00341***. 2023

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

E. M. Sunshine, M. Shuaibi, Z. W. Ulissi, J. R. Kitchin ***arXiv preprint arXiv:2309.04811***. 2023

[64] **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

[63] **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 ***arXiv preprint arXiv:2311.01987***. 2023

[62] **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

[61] **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

[60] **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

[59] **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

[58] **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

[57] **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

[56] **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

[55] **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

[54] **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

[53] **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

[52] **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

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

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

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

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

[49] **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

[48] **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

[47] **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

[46] **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

[45] **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

[44] **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

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

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

[42] **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

[41] **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

[40] **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

[39] **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

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

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

[37] **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

[36] **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

[35] **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

[34] **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

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

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

[32] **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

[31] **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

[30] **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

[29] **Convolutional Neural Network of Atomic Surface Structures To Predict Binding Energies for High-Throughput Screening of Catalysts**

S. Back, J. Yoon, N. Tian, W. Zhong, K. Tran, Z. W. Ulissi ***The Journal of Physical Chemistry Letters*** pp. 4401–4408, 2019

[28] **Theoretical Investigations of Transition Metal Surface Energies under Lattice Strain and CO Environment**

M. T. Tang, Z. W. Ulissi, K. Chan ***The Journal of Physical Chemistry C*** pp. 14481–14487, 2018

[27] **Dynamic workflows for routine materials discovery in surface science**

K. Tran, A. Palizhati, S. Back, Z. W. Ulissi ***Journal of Chemical Information and Modeling*** pp. 2392–2400, 2018

[26] **Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution**

K. Tran, Z. W. Ulissi ***Nature Catalysis*** p. 696, 2018

[25] **Copper Silver Thin Films with Metastable Miscibility for Oxygen Reduction Electrocatalysis in Alkaline Electrolytes**

D. Higgins, M. Wette, B. M. Gibbons, S. Siahrostami, C. Hahn, M. Escudero-Escribano, M. Garcia-Melchor, Z. W. Ulissi, R. C. Davis, A. Mehta, B. M. Clemens, J. K. Nørskov, T. F. Jaramillo ***ACS Applied Energy Materials***. 2018

[24] **Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO2 Reduction**

Z. W. Ulissi, M. T. Tang, J. Xiao, X. Liu, D. A. Torelli, M. Karamad, K. Cummins, C. Hahn, N. S. Lewis, T. F. Jaramillo, K. Chan, J. K. Nørskov ***ACS Catalysis*** pp. 6600–6608, 2017

[23] **To address surface reaction network complexity using scaling relations machine learning and DFT calculations**

Z. W. Ulissi, A. J. Medford, T. Bligaard, J. K. Nørskov ***Nature Communications***. 2017

[22] **Persistently Auxetic Materials: Engineering the Poisson Ratio of 2D Self-Avoiding Membranes under Conditions of Non-Zero Anisotropic Strain**

Z. W. Ulissi, A. Govind Rajan, M. S. Strano ***ACS Nano*** pp. 7542–7549, 2016

[21] **Automated Discovery and Construction of Surface Phase Diagrams using Machine Learning**

Z. W. Ulissi, A. R. Singh, C. Tsai, J. K. Nørskov ***The Journal of Physical Chemistry Letters***. 2016

[20] **A Mathematical Formulation and Solution of the CoPhMoRe Inverse Problem for Helically Wrapping Polymer Corona Phases on Cylindrical Substrates**

G. Bisker, J. Ahn, S. Kruss, Z. W. Ulissi, D. P. Salem, M. S. Strano ***The Journal of Physical Chemistry C***. 2015

[19] **A 2D Equation-of-State Model for Corona Phase Molecular Recognition on Single-Walled Carbon Nanotube and Graphene Surfaces**

Z. W. Ulissi, J. Zhang, V. Sresht, D. Blankschtein, M. S. Strano ***Langmuir*** pp. 628–636, 2015

[18] **Deterministic modelling of carbon nanotube near-infrared solar cells**

D. O. Bellisario, R. M. Jain, Z. W. Ulissi, M. S. Strano ***Energy Environ. Sci.*** pp. 3769–3781, 2014

[17] **Quantitative Theory of Adsorptive Separation for the Electronic Sorting of Single-Walled Carbon Nanotubes**

R. M. Jain, K. Tvrdy, R. Han, Z. W. Ulissi, M. S. Strano ***ACS Nano*** pp. 3367–3379, 2014

[16] **Spatiotemporal Intracellular Nitric Oxide Signaling Captured using Internalized, Near Infrared Fluorescent Carbon Nanotube Nanosensors**

Z. W. Ulissi, F. Sen, X. Gong, S. Sen, N. Iverson, A. A. Boghossian, L. Godoy, G. Wogan, D. Mukhopadhyay, M. S. Strano ***Nano Letters*** pp. 4887–4894, 2014

[15] **Low Dimensional Carbon Materials for Applications in Mass and Energy Transport**

Q. H. Wang, D. O. Bellisario, L. W. Drahushuk, R. M. Jain, S. Kruss, M. P. Landry, S. G. Mahajan, S. F. E. Shimizu, Z. W. Ulissi, M. S. Strano ***Chemistry of Materials*** pp. 172–183, 2014

[14] **Diameter-dependent ion transport through the interior of isolated single-walled carbon nanotubes**

W. Choi, Z. W. Ulissi, S. F. Shimizu, D. O. Bellisario, M. D. Ellison, M. S. Strano ***Nature Communications*** p. 2397, 2013

[13] **Molecular recognition using corona phase complexes made of synthetic polymers adsorbed on carbon nanotubes**

J. Zhang, M. P. Landry, P. W. Barone, J.-H. Kim, S. Lin, Z. W. Ulissi, D. Lin, B. Mu, A. A. Boghossian, A. J. Hilmer, A. Rwei, A. C. Hinckley, S. Kruss, M. A. Shandell, N. Nair, S. Blake, F. Sen, S. Sen, R. G. Croy, D. Li, K. Yum, J.-H. Ahn, H. Jin, D. A. Heller, J. M. Essigmann, D. Blankschtein, M. S. Strano ***Nature Nanotechnology*** pp. 959–968, 2013

[12] **A Quantitative and Predictive Model of Electromigration-Induced Breakdown of Metal Nanowires**

D. O. Bellisario, Z. W. Ulissi, M. S. Strano ***Journal of Physical Chemistry C*** pp. 12373–12378, 2013

[11] **Charge Transfer at Junctions of a Single Layer of Graphene and a Metallic Single Walled Carbon Nanotube**

G. L. C. Paulus, Q. H. Wang, Z. W. Ulissi, T. P. McNicholas, A. Vijayaraghavan, C.-J. Shih, Z. Jin, M. S. Strano ***Small*** pp. 1954–1963, 2013

[10] **Stochastic Pore Blocking and Gating in PDMS-Glass Nanopores from Vapor-Liquid Phase Transitions**

S. Shimizu, M. Ellison, K. Aziz, Q. H. Wang, Z. W. Ulissi, Z. Gunther, D. Bellisario, M. Strano ***Journal of Physical Chemistry C*** pp. 9641–9651, 2013

[9] **Control of nano and microchemical systems**

Z. W. Ulissi, M. S. Strano, R. D. Braatz ***Computers & Chemical Engineering*** pp. 149–156, 2013

[8] **Observation of Oscillatory Surface Reactions of Riboflavin, Trolox, and Singlet Oxygen Using Single Carbon Nanotube Fluorescence Spectroscopy**

F. Sen, A. A. Boghossian, S. Sen, Z. W. Ulissi, J. Zhang, M. S. Strano ***ACS Nano*** pp. 10632–10645, 2012

[7] **Modelling and development of photoelectrochemical reactor for H-2 production**

C. Carver, Z. W. Ulissi, C. K. Ong, S. Dennison, G. H. Kelsall, K. Hellgardt ***International Journal of Hydrogen Energy*** pp. 2911–2923, 2012

[6] **The chemical dynamics of nanosensors capable of single-molecule detection**

A. A. Boghossian, J. Zhang, F. T. Le Floch-Yin, Z. W. Ulissi, P. Bojo, J.-H. Han, J.-H. Kim, J. R. Arkalgud, N. F. Reuel, R. D. Braatz, M. S. Strano ***The Journal of Chemical Physics*** p. 084124, 2011

[5] **Carbon Nanotubes as Molecular Conduits: Advances and Challenges for Transport through Isolated Sub-2 nm Pores**

Z. W. Ulissi, S. Shimizu, C. Y. Lee, M. S. Strano ***Journal of Physical Chemistry Letters*** pp. 2892–2896, 2011

[4] **Effect of multiscale model uncertainty on identification of optimal catalyst properties**

Z. W. Ulissi, V. Prasad, D. Vlachos ***Journal of Catalysis*** pp. 339–344, 2011

[3] **Applicability of Birth-Death Markov Modeling for Single-Molecule Counting Using Single-Walled Carbon Nanotube Fluorescent Sensor Arrays**

Z. W. Ulissi, J. Zhang, A. A. Boghossian, N. F. Reuel, S. F. E. Shimizu, R. D. Braatz, M. S. Strano ***Journal of Physical Chemistry Letters*** pp. 1690–1694, 2011

[2] **High throughput multiscale modeling for design of experiments, catalysts, and reactors: Application to hydrogen production from ammonia**

V. Prasad, A. Karim, Z. W. Ulissi, M. Zagrobelny, D. Vlachos ***Chemical Engineering Science*** pp. 240–246, 2010

[1] **Visualization of biological texture using correlation coefficient images**

A. P. Sviridov, Z. W. Ulissi, V. V. Chernomordik, M. Hassan, A. H. Gandjbakhche ***Journal of Biomedical Optics*** p. 060504, 2006

External Support (CMU)

Toyota Research Institute PI: Zachary Ulissi, Co-PI: Jeffrey Schneider (*2021-2022*)
Meta/Facebook Fundamental AI Research PI: Zachary Ulissi (*2021-2022*)
Army Research Office PI: Zachary Ulissi (*2020-2023*)
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*)
DOE EERE PI: S Litster, Co-PI: A Young, D Paul, B Inci, S Knights, Z Ulissi (*2019 - 2022*)
NSF CBET PI: Andrew Gellman, Co-PI: John Kitchin, Jingguang Chen, Zachary Ulissi (*2019 - 2023*)
DOE NERSC Early Science Application Program for Perlmutter PI: Zachary Ulissi *Post-Doc Support* (*2019 - PRES*)
DOE BES PI: A Peterson, Co-PI: F Goldsmith, B Rubenstein, AJ Medford, Z Ulissi, A Willard (*2018 - 2022*)
DOE OLCF Summit Allocation PI: Zachary Ulissi *35k Node-Hours* (*2021*)
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)