

Zachary W. Ulissi

RESEARCH SCIENTIST · META FUNDAMENTAL AI RESEARCH

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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

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) (2/2023)
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 _____

- [79] **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
- [78] **Adapting OC20-trained EquiformerV2 Models for High-Entropy Materials**
C. M. Clausen, J. Rossmeisl, Z. W. Ulissi *arXiv preprint arXiv:2403.09811*. 2024
- [77] **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
- [76] **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
- [75] **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
- [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. Lori, 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 H₂O₂ 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
- [30] **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
- [29] **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
- [28] **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
- [27] **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
- [26] **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
- [25] **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
- [24] **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
- [23] **Persistently Auxetic Materials: Engineering the Poisson Ratio of 2D Self-Avoiding Membranes under Conditions of Non-Zero Anisotropic Strain**
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Symposia	AIChE Annual Meeting (2018-present), MRS Fall Meeting (2019), CMU/GT Machine Learning in Science in Engineering (2018), ACS Spring Meeting (2018)