Zachary W Ulissi

List of Publications by Year
in descending order

42	3,766	304743	254184
papers	citations	22 h-index	43 g-index

44	44	44	4192
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Heterogeneous Catalysis in Grammar School. Journal of Physical Chemistry C, 2022, 126, 2931-2936.	3.1	4
2	Transfer learning using attentions across atomic systems with graph neural networks (TAAG). Journal of Chemical Physics, 2022, 156, 184702.	3.0	14
3	Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery. ACS Catalysis, 2022, 12, 8572-8581.	11.2	18
4	Enabling robust offline active learning for machine learning potentials using simple physics-based priors. Machine Learning: Science and Technology, 2021, 2, 025007.	5.0	19
5	Elimination of Multidrug-Resistant Bacteria by Transition Metal Dichalcogenides Encapsulated by Synthetic Single-Stranded DNA. ACS Applied Materials & Interfaces, 2021, 13, 8082-8094.	8.0	16
6	Efficient Discovery of Active, Selective, and Stable Catalysts for Electrochemical H₂O₂ Synthesis through Active Motif Screening. ACS Catalysis, 2021, 11, 2483-2491.	11.2	44
7	Computational catalyst discovery: Active classification through myopic multiscale sampling. Journal of Chemical Physics, 2021, 154, 124118.	3.0	7
8	Open Catalyst 2020 (OC20) Dataset and Community Challenges. ACS Catalysis, 2021, 11, 6059-6072.	11.2	201
9	Deep reinforcement learning for predicting kinetic pathways to surface reconstruction in a ternary alloy. Machine Learning: Science and Technology, 2021, 2, 045018.	5.0	14
10	Capturing Structural Transitions in Surfactant Adsorption Isotherms at Solid/Solution Interfaces. Langmuir, 2020, 36, 819-826.	3.5	4
11	Differentiable Optimization for the Prediction of Ground State Structures (DOGSS). Physical Review Letters, 2020, 125, 173001.	7.8	8
12	Discovery of Acid-Stable Oxygen Evolution Catalysts: High-Throughput Computational Screening of Equimolar Bimetallic Oxides. ACS Applied Materials & Interfaces, 2020, 12, 38256-38265.	8.0	47
13	In silico discovery of active, stable, CO-tolerant and cost-effective electrocatalysts for hydrogen evolution and oxidation. Physical Chemistry Chemical Physics, 2020, 22, 19454-19458.	2.8	12
14	Accelerated discovery of CO2 electrocatalysts using active machine learning. Nature, 2020, 581, 178-183.	27.8	807
15	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. ACS Catalysis, 2020, 10, 4244-4252.	11.2	41
16	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. Journal of Physical Chemistry Letters, 2020, 11, 3185-3191.	4.6	63
17	Methods for comparing uncertainty quantifications for material property predictions. Machine Learning: Science and Technology, 2020, 1, 025006.	5.0	78
18	Toward a Design of Active Oxygen Evolution Catalysts: Insights from Automated Density Functional Theory Calculations and Machine Learning. ACS Catalysis, 2019, 9, 7651-7659.	11.2	118

#	Article	IF	Citations
19	Convolutional Neural Network of Atomic Surface Structures To Predict Binding Energies for High-Throughput Screening of Catalysts. Journal of Physical Chemistry Letters, 2019, 10, 4401-4408.	4.6	151
20	Toward Predicting Intermetallics Surface Properties with High-Throughput DFT and Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 4742-4749.	5.4	45
21	Optimization-Based Design of Active and Stable Nanostructured Surfaces. Journal of Physical Chemistry C, 2019, 123, 29209-29218.	3.1	8
22	Dynamic Workflows for Routine Materials Discovery in Surface Science. Journal of Chemical Information and Modeling, 2018, 58, 2392-2400.	5.4	39
23	Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution. Nature Catalysis, 2018, 1, 696-703.	34.4	497
24	Theoretical Investigations of Transition Metal Surface Energies under Lattice Strain and CO Environment. Journal of Physical Chemistry C, 2018, 122, 14481-14487.	3.1	14
25	Copper Silver Thin Films with Metastable Miscibility for Oxygen Reduction Electrocatalysis in Alkaline Electrolytes. ACS Applied Energy Materials, 2018, 1, 1990-1999.	5.1	40
26	To address surface reaction network complexity using scaling relations machine learning and DFT calculations. Nature Communications, 2017, 8, 14621.	12.8	399
27	Machine-Learning Methods Enable Exhaustive Searches for Active Bimetallic Facets and Reveal Active Site Motifs for CO₂ Reduction. ACS Catalysis, 2017, 7, 6600-6608.	11.2	300
28	Automated Discovery and Construction of Surface Phase Diagrams Using Machine Learning. Journal of Physical Chemistry Letters, 2016, 7, 3931-3935.	4.6	74
29	Persistently Auxetic Materials: Engineering the Poisson Ratio of 2D Self-Avoiding Membranes under Conditions of Non-Zero Anisotropic Strain. ACS Nano, 2016, 10, 7542-7549.	14.6	13
30	2D Equation-of-State Model for Corona Phase Molecular Recognition on Single-Walled Carbon Nanotube and Graphene Surfaces. Langmuir, 2015, 31, 628-636.	3.5	22
31	A Mathematical Formulation and Solution of the CoPhMoRe Inverse Problem for Helically Wrapping Polymer Corona Phases on Cylindrical Substrates. Journal of Physical Chemistry C, 2015, 119, 13876-13886.	3.1	40
32	Quantitative Theory of Adsorptive Separation for the Electronic Sorting of Single-Walled Carbon Nanotubes. ACS Nano, 2014, 8, 3367-3379.	14.6	31
33	Low Dimensional Carbon Materials for Applications in Mass and Energy Transport. Chemistry of Materials, 2014, 26, 172-183.	6.7	42
34	Spatiotemporal Intracellular Nitric Oxide Signaling Captured Using Internalized, Near-Infrared Fluorescent Carbon Nanotube Nanosensors. Nano Letters, 2014, 14, 4887-4894.	9.1	91
35	Control of nano and microchemical systems. Computers and Chemical Engineering, 2013, 51, 149-156.	3.8	20
36	Molecular recognition using corona phase complexes made of synthetic polymers adsorbed on carbon nanotubes. Nature Nanotechnology, 2013, 8, 959-968.	31.5	282

#	Article	IF	Citations
37	Charge Transfer at Junctions of a Single Layer of Graphene and a Metallic Single Walled Carbon Nanotube. Small, 2013, 9, 1954-1963.	10.0	24
38	Stochastic Pore Blocking and Gating in PDMSâ€“Glass Nanopores from Vaporâ€“Liquid Phase Transitions. Journal of Physical Chemistry C, 2013, 117, 9641-9651.	3.1	15
39	A Quantitative and Predictive Model of Electromigration-Induced Breakdown of Metal Nanowires. Journal of Physical Chemistry C, 2013, 117, 12373-12378.	3.1	9
40	Observation of Oscillatory Surface Reactions of Riboflavin, Trolox, and Singlet Oxygen Using Single Carbon Nanotube Fluorescence Spectroscopy. ACS Nano, 2012, 6, 10632-10645.	14.6	58
41	Applicability of Birthâ€“Death Markov Modeling for Single-Molecule Counting Using Single-Walled Carbon Nanotube Fluorescent Sensor Arrays. Journal of Physical Chemistry Letters, 2011, 2, 1690-1694.	4.6	11
42	Carbon Nanotubes as Molecular Conduits: Advances and Challenges for Transport through Isolated Sub-2 nm Pores. Journal of Physical Chemistry Letters, 2011, 2, 2892-2896.	4.6	19