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	Accelerated discovery of CO2 electrocatalysts using active machine learning. Nature, 2020, 581, 178-183.	27.8	807
2	Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution. Nature Catalysis, 2018, 1, 696-703.	34.4	497
3	To address surface reaction network complexity using scaling relations machine learning and DFT calculations. Nature Communications, 2017, 8, 14621.	12.8	399
4	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
5	Molecular recognition using corona phase complexes made of synthetic polymers adsorbed on carbon nanotubes. Nature Nanotechnology, 2013, 8, 959-968.	31.5	282
6	Open Catalyst 2020 (OC20) Dataset and Community Challenges. ACS Catalysis, 2021, 11, 6059-6072.	11.2	201
7	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
8	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
9	Spatiotemporal Intracellular Nitric Oxide Signaling Captured Using Internalized, Near-Infrared Fluorescent Carbon Nanotube Nanosensors. Nano Letters, 2014, 14, 4887-4894.	9.1	91
10	Methods for comparing uncertainty quantifications for material property predictions. Machine Learning: Science and Technology, 2020, 1, 025006.	5.0	78
11	Automated Discovery and Construction of Surface Phase Diagrams Using Machine Learning. Journal of Physical Chemistry Letters, 2016, 7, 3931-3935.	4.6	74
12	Practical Deep-Learning Representation for Fast Heterogeneous Catalyst Screening. Journal of Physical Chemistry Letters, 2020, 11, 3185-3191.	4.6	63
13	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
14	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
15	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
16	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
17	Low Dimensional Carbon Materials for Applications in Mass and Energy Transport. Chemistry of Materials, 2014, 26, 172-183.	6.7	42
18	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. ACS Catalysis, 2020, 10, 4244-4252.	11.2	41

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19	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
20	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
21	Dynamic Workflows for Routine Materials Discovery in Surface Science. Journal of Chemical Information and Modeling, 2018, 58, 2392-2400.	5.4	39
22	Quantitative Theory of Adsorptive Separation for the Electronic Sorting of Single-Walled Carbon Nanotubes. ACS Nano, 2014, 8, 3367-3379.	14.6	31
23	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
24	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
25	Control of nano and microchemical systems. Computers and Chemical Engineering, 2013, 51, 149-156.	3.8	20
26	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
27	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
28	Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery. ACS Catalysis, 2022, 12, 8572-8581.	11.2	18
29	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
30	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
31	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
32	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
33	Transfer learning using attentions across atomic systems with graph neural networks (TAAG). Journal of Chemical Physics, 2022, 156, 184702.	3.0	14
34	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
35	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
36	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

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37	A Quantitative and Predictive Model of Electromigration-Induced Breakdown of Metal Nanowires. Journal of Physical Chemistry C, 2013, 117, 12373-12378.	3.1	9
38	Optimization-Based Design of Active and Stable Nanostructured Surfaces. Journal of Physical Chemistry C, 2019, 123, 29209-29218.	3.1	8
39	Differentiable Optimization for the Prediction of Ground State Structures (DOGSS). Physical Review Letters, 2020, 125, 173001.	7.8	8
40	Computational catalyst discovery: Active classification through myopic multiscale sampling. Journal of Chemical Physics, 2021, 154, 124118.	3.0	7
41	Capturing Structural Transitions in Surfactant Adsorption Isotherms at Solid/Solution Interfaces. Langmuir, 2020, 36, 819-826.	3.5	4
42	Heterogeneous Catalysis in Grammar School. Journal of Physical Chemistry C, 2022, 126, 2931-2936.	3.1	4