Tim Mueller

List of Publications by Year
in descending order

45 papers	5,946 citations	147801 31 h-index	233421 45 g-index
48 all docs	48 docs citations	48 times ranked	8697 citing authors

#	Article	IF	Citations
1	High-performance transition metalâ€“doped Pt ₃ Ni octahedra for oxygen reduction reaction. Science, 2015, 348, 1230-1234.	12.6	1,623
2	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
3	Finding Natureâ€™s Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory. Chemistry of Materials, 2010, 22, 3762-3767.	6.7	479
4	Evaluation of Tavorite-Structured Cathode Materials for Lithium-Ion Batteries Using High-Throughput Computing. Chemistry of Materials, 2011, 23, 3854-3862.	6.7	244
5	Ensemble Effect in Bimetallic Electrocatalysts for CO₂ Reduction. Journal of the American Chemical Society, 2019, 141, 16635-16642.	13.7	238
6	Machine learning for interatomic potential models. Journal of Chemical Physics, 2020, 152, 050902.	3.0	207
7	Machine learning for alloys. Nature Reviews Materials, 2021, 6, 730-755.	48.7	202
8	A Density Functional Theory Study of Hydrogen Adsorption in MOF-5. Journal of Physical Chemistry B, 2005, 109, 17974-17983.	2.6	173
9	Roles of Mo Surface Dopants in Enhancing the ORR Performance of Octahedral PtNi Nanoparticles. Nano Letters, 2018, 18, 798-804.	9.1	162
10	Efficient generation of generalized Monkhorst-Pack grids through the use of informatics. Physical Review B, 2016, 93, .	3.2	149
11	Low-Overpotential Electroreduction of Carbon Monoxide Using Copper Nanowires. ACS Catalysis, 2017, 7, 4467-4472.	11.2	137
12	Mechanistic Insights for Low-Overpotential Electroreduction of CO₂ to CO on Copper Nanowires. ACS Catalysis, 2017, 7, 8578-8587.	11.2	106
13	Bayesian approach to cluster expansions. Physical Review B, 2009, 80, .	3.2	98
14	Machine-learned multi-system surrogate models for materials prediction. Npj Computational Materials, 2019, 5, .	8.7	96
15	Substrate-directed synthesis of MoS2 nanocrystals with tunable dimensionality and optical properties. Nature Nanotechnology, 2020, 15, 29-34.	31.5	94
16	Effect of Particle Size on Hydrogen Release from Sodium Alanate Nanoparticles. ACS Nano, 2010, 4, 5647-5656.	14.6	85
17	Differential Surface Elemental Distribution Leads to Significantly Enhanced Stability of PtNi-Based ORR Catalysts. Matter, 2019, 1, 1567-1580.	10.0	82
18	Lithium Ion Conduction in Cathode Coating Materials from On-the-Fly Machine Learning. Chemistry of Materials, 2020, 32, 3741-3752.	6.7	73

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19	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. Chemistry of Materials, 2013, 25, 2064-2074.	6.7	72
20	Ordered Intermetallic Pd₃Bi Prepared by an Electrochemically Induced Phase Transformation for Oxygen Reduction Electrocatalysis. ACS Nano, 2019, 13, 10818-10825.	14.6	72
21	Theoretical Insights into the Effects of Oxidation and Mo-Doping on the Structure and Stability of Ptâ€“Ni Nanoparticles. Nano Letters, 2016, 16, 7748-7754.	9.1	64
22	Effective interactions between theNâ¯Hbond orientations in lithium imide and a proposed ground-state structure. Physical Review B, 2006, 74, .	3.2	60
23	Undercoordinated Active Sites on 4H Gold Nanostructures for CO₂ Reduction. Nano Letters, 2020, 20, 8074-8080.	9.1	46
24	Fast, accurate, and transferable many-body interatomic potentials by symbolic regression. Npj Computational Materials, 2019, 5, .	8.7	45
25	Rational Design of Pt₃Ni Surface Structures for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2015, 119, 17735-17747.	3.1	44
26	The Use of Cluster Expansions To Predict the Structures and Properties of Surfaces and Nanostructured Materials. Journal of Chemical Information and Modeling, 2018, 58, 2401-2413.	5.4	41
27	Exact expressions for structure selection in cluster expansions. Physical Review B, 2010, 82, .	3.2	38
28	Asymmetrical Câ€“C Coupling for Electroreduction of CO on Bimetallic Cuâ€“Pd Catalysts. ACS Catalysis, 2022, 12, 5275-5283.	11.2	35
29	Ab initiodetermination of structure-property relationships in alloy nanoparticles. Physical Review B, 2012, 86, .	3.2	31
30	Origins of hole traps in hydrogenated nanocrystalline and amorphous silicon revealed through machine learning. Physical Review B, 2014, 89, .	3.2	31
31	Mechanisms for hydrogen evolution on transition metal phosphide catalysts and a comparison to Pt(111). Physical Chemistry Chemical Physics, 2019, 21, 24489-24498.	2.8	31
32	Rapid generation of optimal generalized Monkhorst-Pack grids. Computational Materials Science, 2021, 187, 110100.	3.0	25
33	Identifying models of dielectric breakdown strength from high-throughput data via genetic programming. Scientific Reports, 2017, 7, 17594.	3.3	21
34	Investigation of a Quantum Monte Carlo Protocol To Achieve High Accuracy and High-Throughput Materials Formation Energies. Journal of Chemical Theory and Computation, 2017, 13, 1943-1951.	5.3	20
35	Improved Prediction of Nanoalloy Structures by the Explicit Inclusion of Adsorbates in Cluster Expansions. Journal of Physical Chemistry C, 2018, 122, 18040-18047.	3.1	19
36	Ab initiostudy of the low-temperature phases of lithium imide. Physical Review B, 2010, 82, .	3.2	18

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37	Computationally generated maps of surface structures and catalytic activities for alloy phase diagrams. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 22044-22051.	7.1	14
38	Ionic Conduction through Reaction Products at the Electrolyteâ€“Electrode Interface in All-Solid-State Li⁺ Batteries. ACS Applied Materials & Interfaces, 2020, 12, 55510-55519.	8.0	14
39	Materials with the CrVO₄ structure type as candidate superprotonic conductors. RSC Advances, 2019, 9, 31999-32009.	3.6	10
40	Predicting activation energies for vacancy-mediated diffusion in alloys using a transition-state cluster expansion. Physical Review Materials, 2021, 5, .	2.4	7
41	Cluster Expansion Framework for the Sr(Ti1â€“xFex)O3â€“x/2 (0 < x < 1) Mixed Ionic Electronic Conductor: Properties Based on Realistic Configurations. Chemistry of Materials, 2019, 31, 3144-3153.	6.7	6
42	Computational design of double-layer cathode coatings in all-solid-state batteries. Journal of Materials Chemistry A, 2021, 9, 23206-23213.	10.3	4
43	Comment on â€œCluster expansion and the configurational theory of alloysâ€. Physical Review B, 2017, 95, .	3.2	2
44	Conference report: 2018 materials and data science hackathon (MATDAT18). Molecular Systems Design and Engineering, 2019, 4, 462-468.	3.4	2
45	UCLA researchers develop lower-cost, more efficient nanostructures for PEMFCs. Fuel Cells Bulletin, 2015, 2015, 13.	0.1	0