Joseph H Montoya

List of Publications by Year
in descending order

37 papers	6,556 citations	218677 26 h-index	330143 37 g-index
39 all docs	39 docs citations	39 times ranked	9036 citing authors

#	Article	IF	Citations
1	Toward autonomous materials research: Recent progress and future challenges. Applied Physics Reviews, 2022, 9, .	11.3	17
2	Agents for sequential learning using multiple-fidelity data. Scientific Reports, 2022, 12, 4694.	3.3	9
3	Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries. Journal of Chemical Theory and Computation, 2022, 18, 2737-2748.	5.3	7
4	Novel inorganic crystal structures predicted using autonomous simulation agents. Scientific Data, 2022, 9, .	5.3	7
5	Origins of the Instability of Nonprecious Hydrogen Evolution Reaction Catalysts at Open-Circuit Potential. ACS Energy Letters, 2021, 6, 2268-2274.	17.4	44
6	Rational Solid-State Synthesis Routes for Inorganic Materials. Journal of the American Chemical Society, 2021, 143, 9244-9259.	13.7	48
7	Automated Adsorption Workflow for Semiconductor Surfaces and the Application to Zinc Telluride. Journal of Chemical Information and Modeling, 2021, 61, 3908-3916.	5.4	11
8	Autonomous experimentation systems for materials development: A community perspective. Matter, 2021, 4, 2702-2726.	10.0	143
9	Machine learningâ€“accelerated design and synthesis of polyelemental heterostructures. Science Advances, 2021, 7, eabj5505.	10.3	53
10	Two-dimensional forms of robust CO2 reduction photocatalysts. Npj 2D Materials and Applications, 2020, 4, .	7.9	20
11	Predicting aqueous stability of solid with computed Pourbaix diagram using SCAN functional. Npj Computational Materials, 2020, 6, .	8.7	69
12	Autonomous intelligent agents for accelerated materials discovery. Chemical Science, 2020, 11, 8517-8532.	7.4	49
13	Random forest machine learning models for interpretable X-ray absorption near-edge structure spectrum-property relationships. Npj Computational Materials, 2020, 6, .	8.7	94
14	BEEP: A Python library for Battery Evaluation and Early Prediction. SoftwareX, 2020, 11, 100506.	2.6	29
15	A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. ACS Catalysis, 2020, 10, 7495-7511.	11.2	254
16	MaterialNet: A web-based graph explorer for materials science data. Journal of Open Source Software, 2020, 5, 2105.	4.6	5
17	Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery. Nature Communications, 2019, 10, 443.	12.8	125
18	Efficient Pourbaix diagrams of many-element compounds. Physical Chemistry Chemical Physics, 2019, 21, 25323-25327.	2.8	69

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19	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	10.0	19
20	Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO₃ oxides. Physical Chemistry Chemical Physics, 2018, 20, 3813-3818.	2.8	94
21	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
22	Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis. ACS Catalysis, 2018, 8, 4017-4024.	11.2	80
23	Rutile Alloys in the Mnâ€“Sbâ€“O System Stabilize Mn³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	11.2	97
24	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
25	A high-throughput framework for determining adsorption energies on solid surfaces. Npj Computational Materials, 2017, 3, .	8.7	70
26	Materials for solar fuels and chemicals. Nature Materials, 2017, 16, 70-81.	27.5	1,163
27	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
28	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
29	Understanding trends in Câ€“H bond activation in heterogeneous catalysis. Nature Materials, 2017, 16, 225-229.	27.5	387
30	Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxideâ€Đerived Copper. Angewandte Chemie, 2016, 128, 1472-1476.	2.0	39
31	Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxideâ€Đerived Copper. Angewandte Chemie - International Edition, 2016, 55, 1450-1454.	13.8	166
32	Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening. Catalysis Letters, 2016, 146, 718-724.	2.6	18
33	The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations. ChemSusChem, 2015, 8, 2180-2186.	6.8	1,018
34	Theoretical Insights into a CO Dimerization Mechanism in CO₂ Electroreduction. Journal of Physical Chemistry Letters, 2015, 6, 2032-2037.	4.6	606
35	Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting. Physical Chemistry Chemical Physics, 2015, 17, 2634-2640.	2.8	58
36	Electroreduction of Methanediol on Copper. Catalysis Letters, 2013, 143, 631-635.	2.6	21

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37	Insights into Cï£¿C Coupling in CO₂ Electroreduction on Copper Electrodes. ChemCatChem, 2013, 5, 737-742.	3.7	339