Muratahan Aykol

List of Publications by Year
in descending order

51	7,535	159585	189892
papers	citations	30 h-index	50 g-index

66	66	66	8104
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). Jom, 2013, 65, 1501-1509.	1.9	1,461
2	Data-driven prediction of battery cycle life before capacity degradation. Nature Energy, 2019, 4, 383-391.	39.5	1,237
3	The Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. Npj Computational Materials, 2015, 1, .	8.7	1,200
4	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
5	Closed-loop optimization of fast-charging protocols for batteries with machine learning. Nature, 2020, 578, 397-402.	27.8	470
6	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
7	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
8	A machine learning approach for engineering bulk metallic glass alloys. Acta Materialia, 2018, 159, 102-111.	7.9	163
9	High-throughput computational design of cathode coatings for Li-ion batteries. Nature Communications, 2016, 7, 13779.	12.8	145
10	Controlling the Intercalation Chemistry to Design High-Performance Dual-Salt Hybrid Rechargeable Batteries. Journal of the American Chemical Society, 2014, 136, 16116-16119.	13.7	120
11	Machine learning for continuous innovation in battery technologies. Nature Reviews Materials, 2020, 5, 725-727.	48.7	120
12	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
13	Perspectiveâ€"Combining Physics and Machine Learning to Predict Battery Lifetime. Journal of the Electrochemical Society, 2021, 168, 030525.	2.9	107
14	van der Waals Interactions in Layered Lithium Cobalt Oxides. Journal of Physical Chemistry C, 2015, 119, 19053-19058.	3.1	103
15	Thermodynamic Aspects of Cathode Coatings for Lithiumâ€ion Batteries. Advanced Energy Materials, 2014, 4, 1400690.	19.5	99
16	Benchmarking the acceleration of materials discovery by sequential learning. Chemical Science, 2020, 11, 2696-2706.	7.4	83
17	Local environment dependent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi> for accurate thermochemistry of transition metal compounds. Physical Review B, 2014, 90, .	3.2	82
18	Material design of high-capacity Li-rich layered-oxide electrodes: Li₂MnO₃ and beyond. Energy and Environmental Science, 2017, 10, 2201-2211.	30.8	80

#	Article	IF	Citations
19	Active Learning Accelerated Discovery of Stable Iridium Oxide Polymorphs for the Oxygen Evolution Reaction. Chemistry of Materials, 2020, 32, 5854-5863.	6.7	73
20	Suppressing Manganese Dissolution from Lithium Manganese Oxide Spinel Cathodes with Singleâ€Layer Graphene. Advanced Energy Materials, 2015, 5, 1500646.	19.5	72
21	Network analysis of synthesizable materials discovery. Nature Communications, 2019, 10, 2018.	12.8	72
22	The lithiation process and Li diffusion in amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> and Si from first-principles. Electrochimica Acta, 2020, 331, 135344.	5.2	66
23	Revealing the Conversion Mechanism of Transition Metal Oxide Electrodes during Lithiation from First-Principles. Chemistry of Materials, 2017, 29, 9011-9022.	6.7	60
24	Alleviating oxygen evolution from Li-excess oxide materials through theory-guided surface protection. Nature Communications, 2018, 9, 4597.	12.8	56
25	High-Throughput Study of Lattice Thermal Conductivity in Binary Rocksalt and Zinc Blende Compounds Including Higher-Order Anharmonicity. Physical Review X, 2020, 10, .	8.9	55
26	Machine learningâ€“accelerated design and synthesis of polyelemental heterostructures. Science Advances, 2021, 7, eabj5505.	10.3	53
27	Oxidation Protection with Amorphous Surface Oxides: Thermodynamic Insights from Ab Initio Simulations on Aluminum. ACS Applied Materials & Interfaces, 2018, 10, 3039-3045.	8.0	50
28	Autonomous intelligent agents for accelerated materials discovery. Chemical Science, 2020, 11, 8517-8532.	7.4	49
29	Rational Solid-State Synthesis Routes for Inorganic Materials. Journal of the American Chemical Society, 2021, 143, 9244-9259.	13.7	48
30	Nanoclay assisted strengthening of the fiber/matrix interface in functionally filled polyamide 6 composites. Composite Structures, 2010, 92, 2181-2186.	5.8	32
31	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31
32	Solidification behavior, glass forming ability and thermal characteristics of soft magnetic Feâ€“Coâ€“Bâ€“Siâ€“Nbâ€“Cu bulk amorphous alloys. Intermetallics, 2011, 19, 1330-1337.	3.9	30
33	Strategies for accelerating the adoption of materials informatics. MRS Bulletin, 2018, 43, 683-689.	3.5	29
34	BEEP: A Python library for Battery Evaluation and Early Prediction. SoftwareX, 2020, 11, 100506.	2.6	29
35	Effect of (Mo, W) substitution for Nb on glass forming ability and magnetic properties of Feâ€“Co-based bulk amorphous alloys fabricated by centrifugal casting. Journal of Alloys and Compounds, 2011, 509, 2334-2337.	5.5	24
36	Computational Discovery of Liâ€“Mâ€“O Ion Exchange Materials for Lithium Extraction from Brines. Chemistry of Materials, 2018, 30, 6961-6968.	6.7	23

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37	The phase stability network of all inorganic materials. Science Advances, 2020, 6, eaay5606.	10.3	23
38	Layered-Layered-Spinel Cathode Materials Prepared by a High-Energy Ball-Milling Process for Lithium-ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 363-370.	8.0	20
39	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	10.0	19
40	Effect of vanadium on atomic ordering characteristics and anti-phase boundary energies of B2â€“FeCo alloys. Intermetallics, 2010, 18, 893-899.	3.9	17
41	Toward autonomous materials research: Recent progress and future challenges. Applied Physics Reviews, 2022, 9, .	11.3	17
42	Strength of short fiber reinforced polymers: Effect of fiber length distribution. Polymer Composites, 2008, 29, 644-648.	4.6	14
43	Lithium-Ion Cathode/Coating Pairs for Transition Metal Containment. Journal of the Electrochemical Society, 2016, 163, A2054-A2064.	2.9	14
44	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
45	Agents for sequential learning using multiple-fidelity data. Scientific Reports, 2022, 12, 4694.	3.3	9
46	Reflections on one million compounds in the open quantum materials database (OQMD). JPhys Materials, 2022, 5, 031001.	4.2	9
47	Novel inorganic crystal structures predicted using autonomous simulation agents. Scientific Data, 2022, 9, .	5.3	7
48	Continuum Micro-mechanics of Estimating Interfacial Shear Strength in Short Fiber Composites. Composite Interfaces, 2010, 17, 49-58.	2.3	5
49	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.9	5
50	MaterialNet: A web-based graph explorer for materials science data. Journal of Open Source Software, 2020, 5, 2105.	4.6	5
51	Closed-Loop Optimization of Battery Fast Charging Procedures. ECS Meeting Abstracts, 2019, , .	0.0	0