Muratahan Aykol

List of Publications by Year
in descending order

51 papers	7,535 citations	159585 30 h-index	189892 50 g-index
66 all docs	66 docs citations	66 times ranked	8104 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	Reflections on one million compounds in the open quantum materials database (OQMD). JPhys Materials, 2022, 5, 031001.	4.2	9
4	Novel inorganic crystal structures predicted using autonomous simulation agents. Scientific Data, 2022, 9, .	5.3	7
5	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31
6	Perspective—Combining Physics and Machine Learning to Predict Battery Lifetime. Journal of the Electrochemical Society, 2021, 168, 030525.	2.9	107
7	Rational Solid-State Synthesis Routes for Inorganic Materials. Journal of the American Chemical Society, 2021, 143, 9244-9259.	13.7	48
8	Machine learning–accelerated design and synthesis of polyelemental heterostructures. Science Advances, 2021, 7, eabj5505.	10.3	53
9	The lithiation process and Li diffusion in amorphous SiO_2 and Si from first-principles. Electrochimica Acta, 2020, 331, 135344.	5.2	66
10	Ionic Conduction through Reaction Products at the Electrolyte–Electrode Interface in All-Solid-State Li^+ Batteries. ACS Applied Materials & Interfaces, 2020, 12, 55510-55519.	8.0	14
11	Autonomous intelligent agents for accelerated materials discovery. Chemical Science, 2020, 11, 8517-8532.	7.4	49
12	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
13	BEEP: A Python library for Battery Evaluation and Early Prediction. SoftwareX, 2020, 11, 100506.	2.6	29
14	Machine learning for continuous innovation in battery technologies. Nature Reviews Materials, 2020, 5, 725-727.	48.7	120
15	Active Learning Accelerated Discovery of Stable Iridium Oxide Polymorphs for the Oxygen Evolution Reaction. Chemistry of Materials, 2020, 32, 5854-5863.	6.7	73
16	Benchmarking the acceleration of materials discovery by sequential learning. Chemical Science, 2020, 11, 2696-2706.	7.4	83
17	The phase stability network of all inorganic materials. Science Advances, 2020, 6, eaay5606.	10.3	23
18	Closed-loop optimization of fast-charging protocols for batteries with machine learning. Nature, 2020, 578, 397-402.	27.8	470

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19	MaterialNet: A web-based graph explorer for materials science data. Journal of Open Source Software, 2020, 5, 2105.	4.6	5
20	Network analysis of synthesizable materials discovery. Nature Communications, 2019, 10, 2018.	12.8	72
21	Data-driven prediction of battery cycle life before capacity degradation. Nature Energy, 2019, 4, 383-391.	39.5	1,237
22	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	10.0	19
23	Closed-Loop Optimization of Battery Fast Charging Procedures. ECS Meeting Abstracts, 2019, , .	0.0	0
24	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
25	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
26	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
27	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.9	5
28	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
29	Computational Discovery of Liâ€"Mâ€"O Ion Exchange Materials for Lithium Extraction from Brines. Chemistry of Materials, 2018, 30, 6961-6968.	6.7	23
30	Alleviating oxygen evolution from Li-excess oxide materials through theory-guided surface protection. Nature Communications, 2018, 9, 4597.	12.8	56
31	Strategies for accelerating the adoption of materials informatics. MRS Bulletin, 2018, 43, 683-689.	3.5	29
32	A machine learning approach for engineering bulk metallic glass alloys. Acta Materialia, 2018, 159, 102-111.	7.9	163
33	Revealing the Conversion Mechanism of Transition Metal Oxide Electrodes during Lithiation from First-Principles. Chemistry of Materials, 2017, 29, 9011-9022.	6.7	60
34	Material design of high-capacity Li-rich layered-oxide electrodes: Li_2MnO_3 and beyond. Energy and Environmental Science, 2017, 10, 2201-2211.	30.8	80
35	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
36	High-throughput computational design of cathode coatings for Li-ion batteries. Nature Communications, 2016, 7, 13779.	12.8	145

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37	Lithium-Ion Cathode/Coating Pairs for Transition Metal Containment. Journal of the Electrochemical Society, 2016, 163, A2054-A2064.	2.9	14
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 Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. Npj Computational Materials, 2015, 1, .	8.7	1,200
40	Suppressing Manganese Dissolution from Lithium Manganese Oxide Spinel Cathodes with Single‐Layer Graphene. Advanced Energy Materials, 2015, 5, 1500646.	19.5	72
41	van der Waals Interactions in Layered Lithium Cobalt Oxides. Journal of Physical Chemistry C, 2015, 119, 19053-19058.	3.1	103
42	Thermodynamic Aspects of Cathode Coatings for Lithium‐Ion Batteries. Advanced Energy Materials, 2014, 4, 1400690.	19.5	99
43	Local environment dependent $\text{GGA}+U$ for accurate thermochemistry of transition metal compounds. Physical Review B, 2014, 90, .	3.2	82
44	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
45	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
46	Effect of (Mo, W) substitution for Nb on glass forming ability and magnetic properties of Fe–Co-based bulk amorphous alloys fabricated by centrifugal casting. Journal of Alloys and Compounds, 2011, 509, 2334-2337.	5.5	24
47	Solidification behavior, glass forming ability and thermal characteristics of soft magnetic Fe–Co–B–Si–Nb–Cu bulk amorphous alloys. Intermetallics, 2011, 19, 1330-1337.	3.9	30
48	Nanoclay assisted strengthening of the fiber/matrix interface in functionally filled polyamide 6 composites. Composite Structures, 2010, 92, 2181-2186.	5.8	32
49	Effect of vanadium on atomic ordering characteristics and anti-phase boundary energies of B2–FeCo alloys. Intermetallics, 2010, 18, 893-899.	3.9	17
50	Continuum Micro-mechanics of Estimating Interfacial Shear Strength in Short Fiber Composites. Composite Interfaces, 2010, 17, 49-58.	2.3	5
51	Strength of short fiber reinforced polymers: Effect of fiber length distribution. Polymer Composites, 2008, 29, 644-648.	4.6	14