

Accelerating the discovery of materials for clean energy

Nature Reviews Materials

3, 5-20

DOI: [10.1038/s41578-018-0005-z](https://doi.org/10.1038/s41578-018-0005-z)

Citation Report

#	ARTICLE	IF	CITATIONS
1	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	5.3	88
2	Socialization of Industrial Robots: An Innovative Solution to improve Productivity. , 2018, , .		12
3	Towards a continuous formic acid synthesis: a two-step carbon dioxide hydrogenation in flow. Reaction Chemistry and Engineering, 2018, 3, 912-919.	1.9	23
4	Development of bovine serum albuminâ€capsaicin nanoparticles for biotechnological applications. Applied Nanoscience (Switzerland), 2018, 8, 1877-1886.	1.6	7
5	Quantum machine learning for electronic structure calculations. Nature Communications, 2018, 9, 4195.	5.8	99
6	The role of computational results databases in accelerating the discovery of catalysts. Nature Catalysis, 2018, 1, 809-810.	16.1	52
7	Puzzles and confusions in supercapacitor and battery: Theory and solutions. Journal of Power Sources, 2018, 401, 213-223.	4.0	220
8	Efficient Optimization of the Performance of Mn <sup>2+</sup> â€Doped Kesterite Solar Cell: Machine Learning Aided Synthesis of High Efficient Cu <sub>2</sub> (Mn,Zn)Sn(S,Se) <sub>4</sub> Solar Cells. Solar Rrl, 2018, 2, 1800198.	3.1	46
9	Computing Energy. Joule, 2018, 2, 799-800.	11.7	0
10	How To Optimize Materials and Devices <i>via</i> Design of Experiments and Machine Learning: Demonstration Using Organic Photovoltaics. ACS Nano, 2018, 12, 7434-7444.	7.3	219
11	Machine learning for heterogeneous catalyst design and discovery. AIChE Journal, 2018, 64, 2311-2323.	1.8	258
12	Accelerated discovery of stable lead-free hybrid organic-inorganic perovskites via machine learning. Nature Communications, 2018, 9, 3405.	5.8	442
13	Catalyst: The Metaphysics of Chemical Reactivity. Chem, 2018, 4, 1759-1761.	5.8	11
14	Powering catalysis with supercomputers. Nature Catalysis, 2018, 1, 633-634.	16.1	0
15	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	9.9	113
16	Ni-doped cobalt hexacyanoferrate microcubes as battery-type electrodes for aqueous electrolyte-based electrochemical supercapacitors. Journal of Alloys and Compounds, 2019, 806, 1315-1322.	2.8	51
17	Atomistic structure learning. Journal of Chemical Physics, 2019, 151, .	1.2	26
18	A robotic platform for flow synthesis of organic compounds informed by AI planning. Science, 2019, 365, .	6.0	548

#	ARTICLE	IF	CITATIONS
19	Trends in Solid Adsorbent Materials Development for CO <sub>2</sub> Capture. ACS Applied Materials & Interfaces, 2019, 11, 34533-34559.	4.0	215
20	Discovery of new materials using combinatorial synthesis and high-throughput characterization of thin-film materials libraries combined with computational methods. Npj Computational Materials, 2019, 5, .	3.5	186
21	<i>In vitro</i> disease models 4.0 via automation and high-throughput processing. Biofabrication, 2019, 11, 043002.	3.7	20
22	Artificial intelligence for materials discovery. MRS Bulletin, 2019, 44, 538-544.	1.7	60
23	Statistical Analysis and Discovery of Heterogeneous Catalysts Based on Machine Learning from Diverse Published Data. ChemCatChem, 2019, 11, 4537-4547.	1.8	54
24	Multi-component background learning automates signal detection for spectroscopic data. Npj Computational Materials, 2019, 5, .	3.5	21
25	Machine-learning-assisted discovery of polymers with high thermal conductivity using a molecular design algorithm. Npj Computational Materials, 2019, 5, .	3.5	234
26	Virtual Materials Intelligence for Design and Discovery of Advanced Electrocatalysts. ChemPhysChem, 2019, 20, 2946-2955.	1.0	9
27	Machine-learning-assisted thin-film growth: Bayesian optimization in molecular beam epitaxy of SrRuO <sub>3</sub> thin films. APL Materials, 2019, 7, .	2.2	55
28	Silica Restricting the Sulfur Volatilization of Nickel Sulfide for High-Performance Lithium-Ion Batteries. Advanced Energy Materials, 2019, 9, 1901153.	10.2	94
29	Global discovery of stable and non-toxic hybrid organic-inorganic perovskites for photovoltaic systems by combining machine learning method with first principle calculations. Nano Energy, 2019, 66, 104070.	8.2	48
30	Unravelling the effects of oxidation state of interstitial iodine and oxygen passivation on charge trapping and recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite: a time-domain <i>ab initio</i> study. Chemical Science, 2019, 10, 10079-10088.	3.7	44
31	Discovery of blue singlet exciton fission molecules via a high-throughput virtual screening and experimental approach. Journal of Chemical Physics, 2019, 151, 121102.	1.2	24
32	A facile and versatile route to functional poly(propylene) surfaces via UV-curable coatings. Reactive and Functional Polymers, 2019, 144, 104366.	2.0	11
33	Recent advances in nanostructured electrode-electrolyte design for safe and next-generation electrochemical energy storage. Materials Today Nano, 2019, 8, 100057.	2.3	31
34	Rapid Discovery of Ferroelectric Photovoltaic Perovskites and Material Descriptors via Machine Learning. Small Methods, 2019, 3, 1900360.	4.6	76
35	Recent advances in nanomaterial-based synergistic combination cancer immunotherapy. Chemical Society Reviews, 2019, 48, 3771-3810.	18.7	292
36	Experiment Specification, Capture and Laboratory Automation Technology (ESCALATE): a software pipeline for automated chemical experimentation and data management. MRS Communications, 2019, 9, 846-859.	0.8	51

#	ARTICLE	IF	CITATIONS
37	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	4.4	175
38	Fast and interpretable classification of small X-ray diffraction datasets using data augmentation and deep neural networks. Npj Computational Materials, 2019, 5, .	3.5	177
39	Deep learning for molecular design—a review of the state of the art. Molecular Systems Design and Engineering, 2019, 4, 828-849.	1.7	379
40	Miniaturized and Automated Synthesis of Biomolecules—Overview and Perspectives. Advanced Materials, 2019, 31, 1806656.	11.1	15
41	Using artificial intelligence to accelerate materials development. MRS Bulletin, 2019, 44, 335-344.	1.7	16
42	Toward Design of Novel Materials for Organic Electronics. Advanced Materials, 2019, 31, e1808256.	11.1	101
43	High-Temperature and All-Solid-State Flexible Supercapacitors with Excellent Long-Term Stability Based on Porous Polybenzimidazole/Functional Ionic Liquid Electrolyte. ACS Applied Materials & Interfaces, 2019, 11, 17742-17750.	4.0	31
44	Modeling the Structural and Thermal Properties of Loaded Metal—Organic Frameworks. An Interplay of Quantum and Anharmonic Fluctuations. Journal of Chemical Theory and Computation, 2019, 15, 3237-3249.	2.3	22
45	Machine learning for renewable energy materials. Journal of Materials Chemistry A, 2019, 7, 17096-17117.	5.2	207
46	CRYSTAL: a multi-agent AI system for automated mapping of materials™ crystal structures. MRS Communications, 2019, 9, 600-608.	0.8	22
47	Three-Dimensionally Porous Li-Ion and Li-S Battery Cathodes: A Mini Review for Preparation Methods and Energy-Storage Performance. Nanomaterials, 2019, 9, 441.	1.9	12
48	Molecular simulations of carbon-based materials for selected CO2 separation and water treatment processes. Fluid Phase Equilibria, 2019, 492, 10-25.	1.4	19
49	Autonomous Molecular Design: Then and Now. ACS Applied Materials & Interfaces, 2019, 11, 24825-24836.	4.0	69
50	Data-enabled structure—property mappings for lanthanide-activated inorganic scintillators. Journal of Materials Science, 2019, 54, 8361-8380.	1.7	9
51	SLIPS-TENG: robust triboelectric nanogenerator with optical and charge transparency using a slippery interface. National Science Review, 2019, 6, 540-550.	4.6	110
52	Transfer-Learning-Based Coarse-Graining Method for Simple Fluids: Toward Deep Inverse Liquid-State Theory. Journal of Physical Chemistry Letters, 2019, 10, 1242-1250.	2.1	36
53	Dynamic Nanostructures from DNA—Coupled Molecules, Polymers, and Nanoparticles. Small, 2019, 15, e1900504.	5.2	26
54	Recent Advances in Rational Electrode Designs for High-Performance Alkaline Rechargeable Batteries. Advanced Functional Materials, 2019, 29, 1807847.	7.8	152

#	ARTICLE	IF	CITATIONS
55	Concepts for improving hydrogen storage in nanoporous materials. International Journal of Hydrogen Energy, 2019, 44, 7768-7779.	3.8	160
56	Bandgap prediction by deep learning in configurationally hybridized graphene and boron nitride. Npj Computational Materials, 2019, 5, .	3.5	86
57	Automated Multiscale Approach To Predict Self-Diffusion from a Potential Energy Field. Journal of Chemical Theory and Computation, 2019, 15, 2127-2141.	2.3	20
58	Application of hydrides in hydrogen storage and compression: Achievements, outlook and perspectives. International Journal of Hydrogen Energy, 2019, 44, 7780-7808.	3.8	486
59	Solving the electronic structure problem with machine learning. Npj Computational Materials, 2019, 5, .	3.5	191
60	Understanding ML Driven HPC: Applications and Infrastructure. , 2019, , .		2
61	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	5.0	19
62	Progress and prospects for accelerating materials science with automated and autonomous workflows. Chemical Science, 2019, 10, 9640-9649.	3.7	114
63	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	1.3	62
64	Synthesis of nitrogen-doped MnO/carbon network as an advanced catalyst for direct hydrazine fuel cells. Journal of Power Sources, 2019, 413, 209-215.	4.0	41
65	Finding the Right Bricks for Molecular Legos: A Data Mining Approach to Organic Semiconductor Design. Chemistry of Materials, 2019, 31, 969-978.	3.2	38
66	Practical use of polymer brushes in sustainable energy applications: interfacial nanoarchitectonics for high-efficiency devices. Chemical Society Reviews, 2019, 48, 814-849.	18.7	122
67	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 1-4.	2.5	37
68	Autonomous Discovery in the Chemical Sciences Part II: Outlook. Angewandte Chemie - International Edition, 2020, 59, 23414-23436.	7.2	139
69	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. Angewandte Chemie, 2020, 132, 23620-23643.	1.6	4
70	Constrained Bayesian optimization for automatic chemical design using variational autoencoders. Chemical Science, 2020, 11, 577-586.	3.7	159
71	Predicting Thermal Properties of Crystals Using Machine Learning. Advanced Theory and Simulations, 2020, 3, 1900208.	1.3	34
72	Machine Learning Approaches for Thermoelectric Materials Research. Advanced Functional Materials, 2020, 30, 1906041.	7.8	114

#	ARTICLE	IF	CITATIONS
73	Machine Learning for Catalysis Informatics: Recent Applications and Prospects. ACS Catalysis, 2020, 10, 2260-2297.	5.5	309
74	Investigation on platinum loaded multi-walled carbon nanotubes for hydrogen storage applications. International Journal of Hydrogen Energy, 2020, 45, 2967-2974.	3.8	22
75	Machine-learning-driven discovery of polymers molecular structures with high thermal conductivity. International Journal of Heat and Mass Transfer, 2020, 162, 120381.	2.5	33
76	Multiscale Multifactorial Approaches for Engineering Tendon Substitutes. , 2020, , 1-24.		0
77	Lithium-air, lithium-sulfur, and sodium-ion, which secondary battery category is more environmentally friendly and promising based on footprint family indicators?. Journal of Cleaner Production, 2020, 276, 124244.	4.6	27
78	Solid state chemistry for developing better metal-ion batteries. Nature Communications, 2020, 11, 4976.	5.8	125
79	Accelerated design of photovoltaic Ruddlesden-Popper perovskite $\text{Ca}_6\text{Sn}_4\text{S}_{14}$ using machine learning. APL Materials, 2020, 8, .	2.2	9
80	Autonomous materials synthesis by machine learning and robotics. APL Materials, 2020, 8, .	2.2	69
81	Microfluidic Synthesis of Semiconductor Materials: Toward Accelerated Materials Development in Flow. Particle and Particle Systems Characterization, 2020, 37, 2000256.	1.2	31
82	On-the-fly closed-loop materials discovery via Bayesian active learning. Nature Communications, 2020, 11, 5966.	5.8	167
83	Theoretical insights on acceptor-donor dyads for organic photovoltaics. Physical Chemistry Chemical Physics, 2020, 22, 27413-27424.	1.3	1
84	Autonomous Discovery of Battery Electrolytes with Robotic Experimentation and Machine Learning. Cell Reports Physical Science, 2020, 1, 100264.	2.8	80
85	Machine Learning for Polymer Swelling in Liquids. ACS Applied Polymer Materials, 2020, 2, 3576-3586.	2.0	19
86	AI Applications through the Whole Life Cycle of Material Discovery. Matter, 2020, 3, 393-432.	5.0	86
87	Navigating the design space of inorganic materials synthesis using statistical methods and machine learning. Dalton Transactions, 2020, 49, 11480-11488.	1.6	24
88	An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery. Npj Computational Materials, 2020, 6, .	3.5	39
89	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. Physical Chemistry Chemical Physics, 2020, 22, 19326-19341.	1.3	20
90	Machine learning for accelerating the discovery of high-performance donor/acceptor pairs in non-fullerene organic solar cells. Npj Computational Materials, 2020, 6, .	3.5	77

#	ARTICLE	IF	CITATIONS
91	Active Reaction Control of Cu Redox State Based on Real-Time Feedback from In Situ Synchrotron Measurements. <i>Journal of the American Chemical Society</i> , 2020, 142, 18758-18762.	6.6	9
92	Computational discovery of molecular C60 encapsulants with an evolutionary algorithm. <i>Communications Chemistry</i> , 2020, 3, .	2.0	10
93	Autonomous intelligent agents for accelerated materials discovery. <i>Chemical Science</i> , 2020, 11, 8517-8532.	3.7	49
94	Boxing Clever: Robotic Screening of Catalysts Using an Adapted Gas Chromatograph. <i>Matter</i> , 2020, 3, 611-612.	5.0	5
95	Novel Heterogeneous Catalysts for CO <sub>2</sub> Hydrogenation to Liquid Fuels. <i>ACS Central Science</i> , 2020, 6, 1657-1670.	5.3	182
96	Computational Discovery of Stable Heteroanionic Oxychalcogenides ABXO (A, B = Metals; X = S, Se, and Tl) with High Thermodynamic Stability. <i>Chemical Communications</i> , 2020, 11, 11414-11417.	3.2	21
97	Designing and understanding light-harvesting devices with machine learning. <i>Nature Communications</i> , 2020, 11, 4587.	5.8	57
98	DeepGraphMolGen, a multi-objective, computational strategy for generating molecules with desirable properties: a graph convolution and reinforcement learning approach. <i>Journal of Cheminformatics</i> , 2020, 12, 53.	2.8	42
99	Factors Influencing the Development Ability of Intelligent Manufacturing of New Energy Vehicles Based on a Structural Equation Model. <i>ACS Omega</i> , 2020, 5, 18262-18272.	1.6	11
100	Random forest machine learning models for interpretable X-ray absorption near-edge structure spectrum-property relationships. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	94
101	Deep Mining Stable and Nontoxic Hybrid Organic-Inorganic Perovskites for Photovoltaics via Progressive Machine Learning. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 57821-57831.	4.0	20
102	Crystal Site Feature Embedding Enables Exploration of Large Chemical Spaces. <i>Matter</i> , 2020, 3, 433-448.	5.0	33
103	Machine Learning for Materials Scientists: An Introductory Guide toward Best Practices. <i>Chemistry of Materials</i> , 2020, 32, 4954-4965.	3.2	224
104	High-throughput experimentation meets artificial intelligence: a new pathway to catalyst discovery. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11174-11196.	1.3	84
105	Semitransparent Flexible Organic Solar Cells. <i>Chemical Research in Chinese Universities</i> , 2020, 36, 343-350.	1.3	18
106	High-Throughput Screening of Antisolvents for the Deposition of High-Quality Perovskite Thin Films. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 26026-26032.	4.0	11
107	Perspective: Oxygen Separation Technology Based on Liquid-Oxide Electrochemical Membranes. <i>Journal of the Electrochemical Society</i> , 2020, 167, 103501.	1.3	6
108	Materials Acceleration Platforms: On the way to autonomous experimentation. <i>Current Opinion in Green and Sustainable Chemistry</i> , 2020, 25, 100370.	3.2	67

#	ARTICLE	IF	CITATIONS
109	Opportunities and Challenges for Machine Learning in Materials Science. <i>Annual Review of Materials Research</i> , 2020, 50, 71-103.	4.3	183
110	Robot-Accelerated Perovskite Investigation and Discovery. <i>Chemistry of Materials</i> , 2020, 32, 5650-5663.	3.2	113
111	High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	60
112	Exploration of Advanced Electrode Materials for Approaching High-Performance Nickel-Based Superbatteries. <i>Small</i> , 2020, 16, e2001340.	5.2	26
113	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. <i>Chemical Reviews</i> , 2020, 120, 8066-8129.	23.0	284
114	Autonomous molecular design by Monte-Carlo tree search and rapid evaluations using molecular dynamics simulations. <i>Communications Physics</i> , 2020, 3, .	2.0	30
115	Progress in Computational and Machine Learning Methods for Heterogeneous Small-Molecule Activation. <i>Advanced Materials</i> , 2020, 32, e1907865.	11.1	46
116	Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization. <i>ACS Central Science</i> , 2020, 6, 513-524.	5.3	114
117	Predicting the state of charge and health of batteries using data-driven machine learning. <i>Nature Machine Intelligence</i> , 2020, 2, 161-170.	8.3	338
118	Supported and coordinated single metal site electrocatalysts. <i>Materials Today</i> , 2020, 37, 93-111.	8.3	71
119	Cumulative charging behavior of water droplet driven freestanding triboelectric nanogenerators toward hydrodynamic energy harvesting. <i>Journal of Materials Chemistry A</i> , 2020, 8, 7880-7888.	5.2	69
120	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3286-3299.	1.1	48
121	Deep learning and knowledge-based methods for computer-aided molecular design toward a unified approach: State-of-the-art and future directions. <i>Computers and Chemical Engineering</i> , 2020, 141, 107005.	2.0	67
122	A mobile robotic chemist. <i>Nature</i> , 2020, 583, 237-241.	13.7	645
123	Discovery of superionic conductors by ensemble-scope descriptor. <i>NPG Asia Materials</i> , 2020, 12, .	3.8	16
124	Identifying superionic conductors by materials informatics and high-throughput synthesis. <i>Communications Materials</i> , 2020, 1, .	2.9	16
125	Toward "On-Demand" Materials Synthesis and Scientific Discovery through Intelligent Robots. <i>Advanced Science</i> , 2020, 7, 1901957.	5.6	42
126	Embedding physics domain knowledge into a Bayesian network enables layer-by-layer process innovation for photovoltaics. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	18



#	ARTICLE	IF	CITATIONS
127	A microarray platform designed for high-throughput screening the reaction conditions for the synthesis of micro/nanosized biomedical materials. <i>Bioactive Materials</i> , 2020, 5, 286-296.	8.6	10
128	Automation of Active Space Selection for Multireference Methods via Machine Learning on Chemical Bond Dissociation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2389-2399.	2.3	40
129	Optical monitoring of polymerizations in droplets with high temporal dynamic range. <i>Chemical Science</i> , 2020, 11, 2647-2656.	3.7	18
130	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. <i>Advanced Materials</i> , 2020, 32, e1907801.	11.1	138
131	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. <i>Polymers</i> , 2020, 12, 163.	2.0	95
132	Carbon science perspective in 2020: Current research and future challenges. <i>Carbon</i> , 2020, 161, 373-391.	5.4	77
133	Automated in Silico Design of Homogeneous Catalysts. <i>ACS Catalysis</i> , 2020, 10, 2354-2377.	5.5	119
134	A Critical Review of Machine Learning of Energy Materials. <i>Advanced Energy Materials</i> , 2020, 10, 1903242.	10.2	319
135	Toward Accelerated Thermoelectric Materials and Process Discovery. <i>ACS Applied Energy Materials</i> , 2020, 3, 2240-2257.	2.5	75
136	Accelerated Development of Refractory Nanocomposite Solar Absorbers using Bayesian Optimization. <i>MRS Advances</i> , 2020, 5, 1537-1545.	0.5	2
137	The effect of dust accumulation on the cleanliness factor of a parabolic trough solar concentrator. <i>Renewable Energy</i> , 2020, 152, 529-539.	4.3	42
138	High-Throughput Process for the Discovery of Antimicrobial Polymers and Their Upscaled Production via Flow Polymerization. <i>Macromolecules</i> , 2020, 53, 631-639.	2.2	55
139	Catalytic materials and chemistry development using a synergistic combination of machine learning and ab initio methods. <i>Computational Materials Science</i> , 2020, 174, 109474.	1.4	26
140	Machine Learning-Enabled Correlation and Modeling of Multimodal Response of Thin Film to Environment on Macro and Nanoscale Using "Lab-on-a-Chip". <i>Advanced Functional Materials</i> , 2020, 30, 1908010.	7.8	12
141	Materials Informatics Screening of Li-Rich Layered Oxide Cathode Materials with Enhanced Characteristics Using Synthesis Data. <i>Batteries and Supercaps</i> , 2020, 3, 427-438.	2.4	16
142	Self-adaptive FeP@C nanocages for reversible and long-term lithium-ion batteries. <i>Chemical Engineering Journal</i> , 2020, 395, 125124.	6.6	19
143	QSAR without borders. <i>Chemical Society Reviews</i> , 2020, 49, 3525-3564.	18.7	427
144	Mechanoluminescence materials for advanced artificial skin. <i>Science Bulletin</i> , 2020, 65, 1147-1149.	4.3	62

#	ARTICLE	IF	CITATIONS
145	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. ACS Nano, 2020, 14, 6589-6598.	7.3	12
146	Autonomous discovery of optically active chiral inorganic perovskite nanocrystals through an intelligent cloud lab. Nature Communications, 2020, 11, 2046.	5.8	77
147	Discovery of Novel Two-Dimensional Photovoltaic Materials Accelerated by Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 3075-3081.	2.1	35
148	Evolving the Materials Genome: How Machine Learning Is Fueling the Next Generation of Materials Discovery. Annual Review of Materials Research, 2020, 50, 1-25.	4.3	49
149	Toward Excellence of Transition Metal-Based Catalysts for CO <sub>2</sub> Electrochemical Reduction: An Overview of Strategies and Rationales. Small Methods, 2020, 4, 2000033.	4.6	60
150	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	1.1	77
151	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. Machine Learning: Science and Technology, 2021, 2, 01LT01.	2.4	4
152	Review of recent advances of polymer based dielectrics for high-energy storage in electronic power devices from the perspective of target applications. Frontiers of Chemical Science and Engineering, 2021, 15, 18-34.	2.3	25
153	Turning chemistry into information for heterogeneous catalysis. International Journal of Quantum Chemistry, 2021, 121, e26382.	1.0	9
154	Composite anti-scaling membrane made of interpenetrating networks of nanofibers for selective separation of lithium. Journal of Membrane Science, 2021, 618, 118668.	4.1	59
155	Carbon-based transition metal sulfides/selenides nanostructures for electrocatalytic water splitting. Journal of Alloys and Compounds, 2021, 852, 156810.	2.8	58
156	High-throughput characterization of the adiabatic temperature change for magnetocaloric materials. Journal of Materials Science, 2021, 56, 2332-2340.	1.7	9
157	Characterization of AE(TM)2Bi2O9 (AE: Ca, Sr, Ba; TM: Nb, Ta) as oxide ion conductors. Journal of the European Ceramic Society, 2021, 41, 1352-1359.	2.8	0
158	Emerging materials intelligence ecosystems propelled by machine learning. Nature Reviews Materials, 2021, 6, 655-678.	23.3	138
159	Self-Driven Multistep Quantum Dot Synthesis Enabled by Autonomous Robotic Experimentation in Flow. Advanced Intelligent Systems, 2021, 3, 2000245.	3.3	58
160	When artificial intelligence meets building energy efficiency, a review focusing on zero energy building. Artificial Intelligence Review, 2021, 54, 2193-2220.	9.7	31
161	Shedding light on CO <sub>2</sub> : Catalytic synthesis of solar methanol. EcoMat, 2021, 3, e12078.	6.8	13
162	Structural and elastic properties of binary semiconductors from energy gaps. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	2

#	ARTICLE	IF	CITATIONS
163	Off-the-shelf deep learning is not enough, and requires parsimony, Bayesianity, and causality. Npj Computational Materials, 2021, 7, .	3.5	28
164	Deep learning for material synthesis and manufacturing systems: A review. Materials Today: Proceedings, 2021, 46, 3263-3269.	0.9	37
165	Inductive effect as a universal concept to design efficient catalysts for CO <sub>2</sub> electrochemical reduction: electronegativity difference makes a difference. Journal of Materials Chemistry A, 2021, 9, 4626-4647.	5.2	12
166	Toward autonomous design and synthesis of novel inorganic materials. Materials Horizons, 2021, 8, 2169-2198.	6.4	61
167	Accelerating organic solar cell material's discovery: high-throughput screening and <i>big data</i> . Energy and Environmental Science, 2021, 14, 3301-3322.	15.6	51
168	A brief comparative study of the potentialities and limitations of machine-learning algorithms and statistical techniques. E3S Web of Conferences, 2021, 266, 02001.	0.2	6
169	Multiscale Multifactorial Approaches for Engineering Tendon Substitutes. Reference Series in Biomedical Engineering, 2021, , 507-530.	0.1	0
170	Research Progress on Three-Dimensionally Porous Li-Ion and Li-S Battery Cathodes. Advances in Energy and Power Engineering, 2021, 09, 118-131.	0.0	0
171	Elucidating the Full Potential of OPV Materials Utilizing a High-Throughput Robot-Based Platform and Machine Learning. Joule, 2021, 5, 495-506.	11.7	86
172	Self-Driven Multistep Quantum Dot Synthesis Enabled by Autonomous Robotic Experimentation in Flow. Advanced Intelligent Systems, 2021, 3, 2170022.	3.3	0
173	PolyDAT: A Generic Data Schema for Polymer Characterization. Journal of Chemical Information and Modeling, 2021, 61, 1150-1163.	2.5	16
174	Identification of the dominant recombination process for perovskite solar cells based on machine learning. Cell Reports Physical Science, 2021, 2, 100346.	2.8	21
176	Enabling thermal-neutral electrolysis for CO <sub>2</sub> -to-fuel conversions with a hybrid deep learning strategy. Energy Conversion and Management, 2021, 230, 113827.	4.4	23
177	Machine learning made easy for optimizing chemical reactions. Nature, 2021, 590, 40-41.	13.7	13
178	Enabling Circular Economy: The Overlooked Role of Inorganic Materials Chemistry. Chemistry - A European Journal, 2021, 27, 6676-6695.	1.7	6
179	Perspective "Combining Physics and Machine Learning to Predict Battery Lifetime. Journal of the Electrochemical Society, 2021, 168, 030525.	1.3	107
180	Preparation of hollow carbon rods by using ZnO as template for high-performance supercapacitor. Journal of Materials Science: Materials in Electronics, 2021, 32, 8491-8502.	1.1	4
181	Free energy of (Co <sub>x</sub> Mn <sub>1-x</sub> ) <sub>3</sub> O <sub>4</sub> mixed phases from machine-learning-enhanced ab initio calculations. Physical Review Materials, 2021, 5, .	0.9	5

#	ARTICLE	IF	CITATIONS
182	The Value of Watching How Materials Grow: A Multimodal Case Study on Halide Perovskites. <i>Advanced Energy Materials</i> , 2021, 11, 2003534.	10.2	12
183	Perspectiveâ€”Accelerated Discovery of Organic-Inorganic Hybrid Materials via Machine Learning. <i>ECS Journal of Solid State Science and Technology</i> , 2021, 10, 037001.	0.9	1
184	A contemporary approach to the MSE paradigm powered by Artificial Intelligence from a review focused on Polymer Matrix Composites. <i>Mechanics of Advanced Materials and Structures</i> , 2022, 29, 3076-3096.	1.5	9
185	Designing heat transfer pathways for advanced thermoregulatory textiles. <i>Materials Today Physics</i> , 2021, 17, 100342.	2.9	44
186	Fibre-based composites from the integration of metalâ€”organic frameworks and polymers. <i>Nature Reviews Materials</i> , 2021, 6, 605-621.	23.3	128
187	Reaction kinetics in rechargeable zinc-ion batteries. <i>Journal of Power Sources</i> , 2021, 492, 229655.	4.0	48
188	Efficient few-shot machine learning for classification of EBSD patterns. <i>Scientific Reports</i> , 2021, 11, 8172.	1.6	17
189	Intensified Energy Storage in High-Voltage Nanohybrid Supercapacitors <i>via</i> the Efficient Coupling between $\text{TiNb}_2\text{O}_7/\text{Holey-rGO}$ Nanoarchitectures and Ionic Liquid-Based Electrolytes. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 21349-21361.	4.0	18
190	Density Prediction Models for Energetic Compounds Merely Using Molecular Topology. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2582-2593.	2.5	25
191	Novel bismuth oxy hydride chromate ( $\text{HBi}_3(\text{CrO}_4)_3$ ) nano-sheets/rods synthesized by one step one pot wet chemical method. <i>IOP SciNotes</i> , 0, , .	0.4	1
192	Toward smart carbon capture with machine learning. <i>Cell Reports Physical Science</i> , 2021, 2, 100396.	2.8	38
193	Machine learning assisted rediscovery of methane storage and separation in porous carbon from material literature. <i>Fuel</i> , 2021, 290, 120080.	3.4	11
194	Toward autonomous additive manufacturing: Bayesian optimization on a 3D printer. <i>MRS Bulletin</i> , 2021, 46, 566-575.	1.7	48
195	Recent progress in conjugated microporous polymers for clean energy: Synthesis, modification, computer simulations, and applications. <i>Progress in Polymer Science</i> , 2021, 115, 101374.	11.8	117
196	Theoretical and computational methods for accelerated materials discovery. <i>Modern Physics Letters B</i> , 2021, 35, 2130003.	1.0	6
197	Machine-learned potentials for next-generation matter simulations. <i>Nature Materials</i> , 2021, 20, 750-761.	13.3	214
198	Theorists and experimentalists must join forces. <i>Nature Computational Science</i> , 2021, 1, 299-299.	3.8	3
199	Dimensionality reduction of complex reaction networks in heterogeneous catalysis: From $\text{linear scaling}$ relationships to statistical learning techniques. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1540.	6.2	10

#	ARTICLE	IF	CITATIONS
200	Review-Emerging Applications of g-C3N4 Films in Perovskite-Based Solar Cells. ECS Journal of Solid State Science and Technology, 0, , .	0.9	10
201	Open Catalyst 2020 (OC20) Dataset and Community Challenges. ACS Catalysis, 2021, 11, 6059-6072.	5.5	201
202	Machine learning the quantum-chemical properties of metal-organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
203	Nobel Turing Challenge: creating the engine for scientific discovery. Npj Systems Biology and Applications, 2021, 7, 29.	1.4	31
204	Artificial neural network modified constitutive descriptions for hot deformation and kinetic models for dynamic recrystallization of novel AZE311 and AZX311 alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2021, 816, 141259.	2.6	23
205	Machine learning in materials science: From explainable predictions to autonomous design. Computational Materials Science, 2021, 193, 110360.	1.4	103
206	An open-source technology platform to increase reproducibility and enable high-throughput production of tailorable gelatin methacryloyl (GelMA) - based hydrogels. Materials and Design, 2021, 204, 109619.	3.3	10
207	Real-Time and Online Lubricating Oil Condition Monitoring Enabled by Triboelectric Nanogenerator. ACS Nano, 2021, 15, 11869-11879.	7.3	56
208	Accelerating Optimizing the Design of Carbon-based Electrocatalyst via Machine Learning. Electroanalysis, 2022, 34, 599-607.	1.5	9
209	Computational sustainability meets materials science. Nature Reviews Materials, 2021, 6, 645-647.	23.3	8
211	Predicting Perovskite Performance with Multiple Machine-Learning Algorithms. Crystals, 2021, 11, 818.	1.0	9
212	Autonomous reinforcement learning agent for chemical vapor deposition synthesis of quantum materials. Npj Computational Materials, 2021, 7, .	3.5	14
213	A Meta-Analysis of Conductive and Strong Carbon Nanotube Materials. Advanced Materials, 2021, 33, e2008432.	11.1	72
214	The Advantage of Nanowire Configuration in Band Structure Determination. Advanced Functional Materials, 2021, 31, 2105426.	7.8	4
215	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	2.4	31
216	Computer aided drug discovery review for infectious diseases with case study of anti-Chagas project. Parasitology International, 2021, 83, 102366.	0.6	3
217	Integration of data-intensive, machine learning and robotic experimental approaches for accelerated discovery of catalysts in renewable energy-related reactions. Materials Reports Energy, 2021, 1, 100049.	1.7	7
218	Recent developments in polydopamine-based photocatalytic nanocomposites for energy production: Physico-chemical properties and perspectives. Catalysis Today, 2022, 397-399, 316-349.	2.2	26

#	ARTICLE	IF	CITATIONS
219	Machine Learning in Chemical Product Engineering: The State of the Art and a Guide for Newcomers. Processes, 2021, 9, 1456.	1.3	28
220	Aggressively optimizing validation statistics can degrade interpretability of data-driven materials models. Journal of Chemical Physics, 2021, 155, 054105.	1.2	10
221	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	2.0	94
222	Semiconductor quantum dots: Technological progress and future challenges. Science, 2021, 373, .	6.0	600
223	Multiscale modelling for fusion and fission materials: The M4F project. Nuclear Materials and Energy, 2021, 29, 101051.	0.6	12
224	Materials-Genome Approach to Energetic Materials. Accounts of Materials Research, 2021, 2, 692-696.	5.9	22
225	Computational discovery of energy materials in the era of big data and machine learning: A critical review. Materials Reports Energy, 2021, 1, 100047.	1.7	24
226	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	23.0	384
227	Extrapolative Bayesian Optimization with Gaussian Process and Neural Network Ensemble Surrogate Models. Advanced Intelligent Systems, 2021, 3, 2100101.	3.3	23
228	Use of metamodels for rapid discovery of narrow bandgap oxide photocatalysts. IScience, 2021, 24, 103068.	1.9	17
229	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	5.5	61
230	Automating crystal-structure phase mapping by combining deep learning with constraint reasoning. Nature Machine Intelligence, 2021, 3, 812-822.	8.3	29
231	Autonomous experimentation systems for materials development: A community perspective. Matter, 2021, 4, 2702-2726.	5.0	143
232	Molecular Dynamics and Machine Learning in Catalysts. Catalysts, 2021, 11, 1129.	1.6	15
233	High-throughput rapid experimental alloy development (HT-READ). Acta Materialia, 2021, 221, 117352.	3.8	23
234	Emerging Zn Anodeâ€Based Electrochromic Devices. Small Science, 2021, 1, 2100040.	5.8	35
236	Phaseâ€Property Diagrams for Multicomponent Oxide Systems toward Materials Libraries. Advanced Materials, 2021, 33, e2102301.	11.1	29
237	Studies on the regularity of perovskite formation via machine learning. Computational Materials Science, 2021, 199, 110712.	1.4	17

#	ARTICLE	IF	CITATIONS
238	A Machine Learning Shortcut for Screening the Spinel Structures of Mg/Zn Ion Battery Cathodes with a High Conductivity and Rapid Ion Kinetics. <i>Energy Storage Materials</i> , 2021, 42, 277-285.	9.5	18
239	Accelerated AI development for autonomous materials synthesis in flow. <i>Chemical Science</i> , 2021, 12, 6025-6036.	3.7	35
240	Determining usefulness of machine learning in materials discovery using simulated research landscapes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14156-14163.	1.3	13
241	Up-scalable emerging energy conversion technologies enabled by 2D materials: from miniature power harvesters towards grid-connected energy systems. <i>Energy and Environmental Science</i> , 2021, 14, 3352-3392.	15.6	26
242	Nonlinear optical probes of nucleation and crystal growth: recent progress and future prospects. <i>Journal of Materials Chemistry C</i> , 2021, 9, 11553-11568.	2.7	8
243	Generative Models for Automatic Chemical Design. <i>Lecture Notes in Physics</i> , 2020, , 445-467.	0.3	42
244	A scrap-tolerant alloying concept based on high entropy alloys. <i>Acta Materialia</i> , 2020, 200, 735-744.	3.8	21
245	Recent progress of biomass-derived carbon materials for supercapacitors. <i>Journal of Power Sources</i> , 2020, 451, 227794.	4.0	290
246	Closed-loop optimization of fast-charging protocols for batteries with machine learning. <i>Nature</i> , 2020, 578, 397-402.	13.7	470
247	Chapter 6. A Prediction of Future States: AI-powered Chemical Innovation for Defense Applications. <i>RSC Theoretical and Computational Chemistry Series</i> , 2020, , 136-168.	0.7	1
248	Deep learning and generative methods in cheminformatics and chemical biology: navigating small molecule space intelligently. <i>Biochemical Journal</i> , 2020, 477, 4559-4580.	1.7	29
249	A machine learning workflow for 4D printing: understand and predict morphing behaviors of printed active structures. <i>Smart Materials and Structures</i> , 2021, 30, 015028.	1.8	17
251	Classification of local chemical environments from x-ray absorption spectra using supervised machine learning. <i>Physical Review Materials</i> , 2019, 3, .	0.9	66
252	Electrospun nanofibers: role of nanofibers in water remediation and effect of experimental variables on their nano topography and application processes. <i>Environmental Science: Water Research and Technology</i> , 2021, 7, 2166-2205.	1.2	6
253	Recent advances in autonomous synthesis of materials. <i>ChemPhysMater</i> , 2022, 1, 77-85.	1.4	11
254	Machine learning for high-throughput experimental exploration of metal halide perovskites. <i>Joule</i> , 2021, 5, 2797-2822.	11.7	44
255	Machine-Learning-Guided Discovery of <sup>19</sup> F MRI Agents Enabled by Automated Copolymer Synthesis. <i>Journal of the American Chemical Society</i> , 2021, 143, 17677-17689.	6.6	66
256	Machine learning in solid heterogeneous catalysis: Recent developments, challenges and perspectives. <i>Chemical Engineering Science</i> , 2022, 248, 117224.	1.9	51



#	ARTICLE	IF	CITATIONS
257	High-Entropy Energy Materials in the Age of Big Data: A Critical Guide to Next-Generation Synthesis and Applications. <i>Advanced Energy Materials</i> , 2021, 11, 2102355.	10.2	37
258	Bayesian learning for rapid prediction of lithium-ion battery-cycling protocols. <i>Joule</i> , 2021, 5, 3187-3203.	11.7	51
259	Accelerate Synthesis of Metal-Organic Frameworks by a Robotic Platform and Bayesian Optimization. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 53485-53491.	4.0	28
260	Identification of Microstructures in 3-Printed Ti-6Al-4V Using Acoustic Emission Cepstrum. <i>Smart and Sustainable Manufacturing Systems</i> , 2020, 4, 163-178.	0.3	4
262	High-Throughput Computational Studies in Catalysis and Materials Research, and Their Impact on Rational Design. , 2020, , 1-44.		1
263	Robotic fabrication of high-quality lamellae for aberration-corrected transmission electron microscopy. <i>Scientific Reports</i> , 2021, 11, 21599.	1.6	5
264	Recommendations for Advancing FAIR and Open Data Standards in the Water Treatment Community. <i>ACS ES&amp;T Engineering</i> , 2022, 2, 337-346.	3.7	6
265	Discovering New Chemistry with an Autonomous Robotic Platform Driven by a Reactivity-Seeking Neural Network. <i>ACS Central Science</i> , 2021, 7, 1821-1830.	5.3	32
266	Mie Sensing with Neural Networks: Recognition of Nano-Object Parameters, the Invisibility Point, and Restricted Models. <i>Advanced Theory and Simulations</i> , 0, , 2100369.	1.3	3
267	Rational Design of Graphene Derivatives for Electrochemical Reduction of Nitrogen to Ammonia. <i>ACS Nano</i> , 2021, 15, 17275-17298.	7.3	48
268	Current Topics in Ionic Liquid Crystals. <i>ChemPlusChem</i> , 2022, 87, .	1.3	47
269	Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data. <i>Nature Communications</i> , 2021, 12, 6595.	5.8	55
270	Modern nanoscience: Convergence of AI, robotics, and colloidal synthesis. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	18
271	Machine Learning-Assisted Computational Screening of Metal-Organic Frameworks for Atmospheric Water Harvesting. <i>Nanomaterials</i> , 2022, 12, 159.	1.9	6
272	Authentic Intelligent Machine for Scaling Driven Discovery: A Case for Chiral Quantum Dots. <i>ACS Nano</i> , 2022, 16, 1600-1611.	7.3	4
273	From Platform to Knowledge Graph: Evolution of Laboratory Automation. <i>Jacs Au</i> , 2022, 2, 292-309.	3.6	42
274	Role of Computational Science in Materials and Systems Design for Sustainable Energy Applications: An Industry Perspective. <i>Journal of the Indian Institute of Science</i> , 2022, 102, 11-37.	0.9	1
275	Effect of substitutional doping and disorder on the phase stability, magnetism, and half-metallicity of Heusler alloys. <i>Acta Materialia</i> , 2022, 225, 117477.	3.8	12



#	ARTICLE	IF	CITATIONS
276	Implementation of Dynamic Controls for Grid-Tied-Inverters through Next-Generation Smart Meters and Its Application in Modernized Grid. <i>Energies</i> , 2022, 15, 988.	1.6	11
277	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials. <i>Nature Communications</i> , 2022, 13, 68.	5.8	48
278	The Solution is the Solution: Data-Driven Elucidation of Solution-to-Device Feature Transfer for $\pi$ -Conjugated Polymer Semiconductors. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 3613-3620.	4.0	16
279	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	70
280	Screening and Understanding Lattice Silicon-Controlled Catalytically Active Site Motifs from a Library of Transition Metal-Silicon Intermetallics. <i>Small</i> , 2022, 18, e2107371.	5.2	12
281	Routescore: Punching the Ticket to More Efficient Materials Development. <i>ACS Central Science</i> , 2022, 8, 122-131.	5.3	8
282	MOF Synthesis Prediction Enabled by Automatic Data Mining and Machine Learning**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	59
283	Review of computational approaches to predict the thermodynamic stability of inorganic solids. <i>Journal of Materials Science</i> , 2022, 57, 10475-10498.	1.7	39
284	The materials tetrahedron has a "digital twin". <i>MRS Bulletin</i> , 2022, 47, 379-388.	1.7	17
285	MOF Synthesis Prediction Enabled by Automatic Data Mining and Machine Learning. <i>Angewandte Chemie</i> , 0, , .	1.6	1
286	Toward autonomous materials research: Recent progress and future challenges. <i>Applied Physics Reviews</i> , 2022, 9, .	5.5	17
287	Electrochromic 2,5-Dihydroxyterephthalic Acid Linker in Metal-Organic Frameworks. <i>Advanced Photonics Research</i> , 0, , 2100219.	1.7	1
288	Application of Advanced Vibrational Spectroscopy in Revealing Critical Chemical Processes and Phenomena of Electrochemical Energy Storage and Conversion. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 23033-23055.	4.0	12
290	Structure-property correlation in oxide-ion and proton conductors for clean energy applications: recent experimental and computational advancements. <i>Journal of Materials Chemistry A</i> , 2022, 10, 5082-5110.	5.2	23
291	Extended DeepLST for Various Thermodynamic States and Applications in Coarse-Graining. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1562-1570.	1.1	6
292	A self-driving laboratory advances the Pareto front for material properties. <i>Nature Communications</i> , 2022, 13, 995.	5.8	55
293	Forecasting the outcome of spintronic experiments with Neural Ordinary Differential Equations. <i>Nature Communications</i> , 2022, 13, 1016.	5.8	17
294	Machine learning in energy storage materials. , 2022, 1, 175-195.		45

#	ARTICLE	IF	CITATIONS
295	Materials, physics and systems for multicaloric cooling. <i>Nature Reviews Materials</i> , 2022, 7, 633-652.	23.8	89
296	Scale-invariant machine-learning model accelerates the discovery of quaternary chalcogenides with ultralow lattice thermal conductivity. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	18
297	Inverse Design of Nanoclusters for Light-Controlled CO <sub>2</sub> →HCOOH Interconversion. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2523-2532.	2.1	3
298	Research on the Operational Strategy of the Hybrid Wind/PV/Small-Hydropower/Facility-Agriculture System Based on a Microgrid. <i>Energies</i> , 2022, 15, 2466.	1.6	4
299	Materials for Sustainable Nuclear Energy: A European Strategic Research and Innovation Agenda for All Reactor Generations. <i>Energies</i> , 2022, 15, 1845.	1.6	13
300	New black indium oxide tandem photothermal CO <sub>2</sub> -H <sub>2</sub> methanol selective catalyst. <i>Nature Communications</i> , 2022, 13, 1512.	5.8	47
301	Multi-objective optimizations of solid oxide co-electrolysis with intermittent renewable power supply via multi-physics simulation and deep learning strategy. <i>Energy Conversion and Management</i> , 2022, 258, 115560.	4.4	9
302	Materials structure-property factorization for identification of synergistic phase interactions in complex solar fuels photoanodes. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	3
303	Unsupervised machine learning to classify crystal structures according to their structural distortion: A case study on Li-argyrodite solid-state electrolytes. <i>Energy and AI</i> , 2022, 9, 100159.	5.8	3
304	Growth of mixed anodic films on combinatorial Al-Gd alloys and their superimposed potential-pH diagrams. <i>Journal of Electroanalytical Chemistry</i> , 2022, 911, 116227.	1.9	1
305	Integration of machine learning and first principles models. <i>AIChE Journal</i> , 2022, 68, .	1.8	23
306	Socially-Directed Development of Materials for Structural Color. <i>Advanced Materials</i> , 2022, 34, e2100939.	11.1	14
307	Nanochannels for low-grade energy harvesting. <i>Current Opinion in Electrochemistry</i> , 2022, 33, 100956.	2.5	2
308	A quantitative permittivity model for designing electromagnetic wave absorption materials with conduction loss: A case study with microwave-reduced graphene oxide. <i>Chemical Engineering Journal</i> , 2022, 439, 135672.	6.6	26
309	A universal, green, and self-reliant electrolytic approach to high-entropy layered (oxy)hydroxide nanosheets for efficient electrocatalytic water oxidation. <i>Journal of Colloid and Interface Science</i> , 2022, 617, 500-510.	5.0	10
310	Stable Room Temperature Thermoelectric Properties in a Supramolecular Assembly of an n-Type Naphthalene-imide-based Amphiphile. <i>ChemNanoMat</i> , 2022, 8, .	1.5	4
311	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams. <i>Science Advances</i> , 2021, 7, eabg4930.	4.7	26
312	Data-Centric Architecture for Self-Driving Laboratories with Autonomous Discovery of New Nanomaterials. <i>Nanomaterials</i> , 2022, 12, 12.	1.9	7

#	ARTICLE	IF	CITATIONS
313	Discovery of Lead-Free Perovskites for High-Performance Solar Cells via Machine Learning: Ultrabroadband Absorption, Low Radiative Combination, and Enhanced Thermal Conductivities. <i>Advanced Science</i> , 2022, 9, e2103648.	5.6	35
314	Sodium-ion battery from sea salt: a review. <i>Materials for Renewable and Sustainable Energy</i> , 2022, 11, 71-89.	1.5	13
315	Data-Driven Materials Innovation and Applications. <i>Advanced Materials</i> , 2022, 34, e2104113.	11.1	51
316	Prospects and challenges for autonomous catalyst discovery viewed from an experimental perspective. <i>Catalysis Science and Technology</i> , 2022, 12, 3650-3669.	2.1	9
317	Accelerating materials discovery using artificial intelligence, high performance computing and robotics. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	71
318	Artificial intelligence modeling of ultrasonic fatigue test to predict the temperature increase. <i>International Journal of Fatigue</i> , 2022, 163, 106999.	2.8	7
319	Opportunities for machine learning to accelerate halide-perovskite commercialization and scale-up. <i>Matter</i> , 2022, 5, 1353-1366.	5.0	8
320	Fast evaluation technique for the shear viscosity and ionic conductivity of electrolyte solutions. <i>Scientific Reports</i> , 2022, 12, 7291.	1.6	1
321	On-the-fly autonomous control of neutron diffraction via physics-informed Bayesian active learning. <i>Applied Physics Reviews</i> , 2022, 9, 021408.	5.5	25
322	Artificial Intelligence for Electricity Supply Chain automation. <i>Renewable and Sustainable Energy Reviews</i> , 2022, 163, 112459.	8.2	21
323	Water electrolysis: from textbook knowledge to the latest scientific strategies and industrial developments. <i>Chemical Society Reviews</i> , 2022, 51, 4583-4762.	18.7	453
324	A novel intelligent strategy-based thermodynamic modeling and analysis of solar-assisted vapor absorption refrigeration system. <i>Environmental Science and Pollution Research</i> , 2022, 29, 71518-71533.	2.7	2
325	Forecasting Carbon Nanotube Diameter in Floating Catalyst Chemical Vapor Deposition. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
326	Accelerating research on novel photovoltaic materials. <i>Faraday Discussions</i> , 0, 239, 235-249.	1.6	2
327	Finding a novel electrolyte solution of lithium-ion batteries using an autonomous search system based on ensemble optimization. <i>Journal of Power Sources</i> , 2022, 541, 231698.	4.0	4
328	Autonomous materials discovery and manufacturing (AMDM): A review and perspectives. <i>IIEE Transactions</i> , 2023, 55, 75-93.	1.6	5
329	Modelling Interfaces in Thin-Film Photovoltaic Devices. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
330	Crystallographic Design of Intercalation Materials. <i>Journal of Electrochemical Energy Conversion and Storage</i> , 0, , 1-23.	1.1	4

#	ARTICLE	IF	CITATIONS
331	Data-Driven Mapping of Inorganic Chemical Space for the Design of Transition Metal Complexes and Metal-Organic Frameworks. ACS Symposium Series, 0, , 127-179.	0.5	0
332	Alloy Profusion, Spice Metals, and Resource Loss by Design. Sustainability, 2022, 14, 7535.	1.6	7
333	Recent progress in 2D hybrid heterostructures from transition metal dichalcogenides and organic layers: properties and applications in energy and optoelectronics fields. Nanoscale, 2022, 14, 10648-10689.	2.8	20
334	Toward Automated Computational Discovery of Battery Materials. Advanced Materials Technologies, 2023, 8, .	3.0	5
335	Electron transfer dominated triboelectrification at the hydrophobic/slippy substrateâ€”water interfaces. Friction, 0, , .	3.4	2
336	Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. Chemical Reviews, 2022, 122, 13478-13515.	23.0	120
337	Challenges and opportunities in carbon capture, utilization and storage: A process systems engineering perspective. Computers and Chemical Engineering, 2022, 166, 107925.	2.0	25
338	Self-Powered, Long-Durable, and Highly Selective Oilâ€”Solid Triboelectric Nanogenerator for Energy Harvesting and Intelligent Monitoring. Nano-Micro Letters, 2022, 14, .	14.4	23
339	Assessing the correlation between the sustainable energy for all with doing a business by artificial neural network. Neural Computing and Applications, 0, , .	3.2	0
340	Rapidly predicting Kohnâ€”Sham total energy using data-centric AI. Scientific Reports, 2022, 12, .	1.6	5
341	Bayesian optimization with experimental failure for high-throughput materials growth. Npj Computational Materials, 2022, 8, .	3.5	9
342	Artificial Intelligenceâ€”Based Material Discovery for Clean Energy Future. Advanced Intelligent Systems, 2022, 4, .	3.3	9
343	Human- and machine-centred designs of molecules and materials for sustainability and decarbonization. Nature Reviews Materials, 2022, 7, 991-1009.	23.3	30
344	An all-round AI-Chemist with a scientific mind. National Science Review, 2022, 9, .	4.6	46
345	A diversity maximizing active learning strategy for graph neural network models of chemical properties. Molecular Systems Design and Engineering, 2022, 7, 1697-1706.	1.7	1
346	Phosphorus-modified Pt@Cu surfaces for efficient electrocatalysis of hydrogen evolution. Materials Advances, 2022, 3, 7667-7672.	2.6	0
347	Forecasting carbon nanotube diameter in floating catalyst chemical vapor deposition. Carbon, 2023, 201, 719-733.	5.4	4
348	Quantum Dot-based Luminescent Solar Concentrators Fabricated through the Ultrasonic Spray-Coating Method. ACS Applied Materials & Interfaces, 2022, 14, 41013-41021.	4.0	9

#	ARTICLE	IF	CITATIONS
349	Battery Materials Discovery and Smart Grid Management using Machine Learning. Batteries and Supercaps, 2022, 5, .	2.4	2
350	Scenarios of the alternative energetics development in the age of the fourth industrial revolution: Clean energy prospects and policy implications. Frontiers in Energy Research, 0, 10, .	1.2	1
351	Principles of the Battery Data Genome. Joule, 2022, 6, 2253-2271.	11.7	26
352	Automatic Evolution of Machine-Learning-Based Quantum Dynamics with Uncertainty Analysis. Journal of Chemical Theory and Computation, 2022, 18, 5837-5855.	2.3	6
353	Augmented Experiment in Material Engineering Using Machine Learning. Proceedings of the AAAI Conference on Artificial Intelligence, 2021, 35, 9251-9258.	3.6	0
354	Machine Learning in the Development of Adsorbents for Clean Energy Application and Greenhouse Gas Capture. Advanced Science, 2022, 9, .	5.6	8
355	A perspective on Bayesian methods applied to materials discovery and design. MRS Communications, 2022, 12, 1037-1049.	0.8	6
356	Review of vanadium and its redox flow batteries for renewable energy storage. Proceedings of Institution of Civil Engineers: Energy, 2024, 177, 3-13.	0.5	1
357	Networks and interfaces as catalysts for polymer materials innovation. Cell Reports Physical Science, 2022, 3, 101126.	2.8	5
358	Toward autonomous laboratories: Convergence of artificial intelligence and experimental automation. Progress in Materials Science, 2023, 132, 101043.	16.0	19
359	Discovery of chalcogenides structures and compositions using mixed fluxes. Nature, 2022, 612, 72-77.	13.7	20
360	Computerized Prediction of Perovskite Performance Using Deep Learning. Electronics (Switzerland), 2022, 11, 3759.	1.8	0
361	è†ªåŠ“åŒ–å’Œæ™ºèf1/2åŒ–çš,,åŒ–å– å•æ•; Scientia Sinica Chimica, 2022, , .	0.2	0
362	Recent developments in the application of machine-learning towards accelerated predictive multiscale design and additive manufacturing. Virtual and Physical Prototyping, 2023, 18, .	5.3	13
363	Robotised screening and characterisation for accelerated discovery of novel Lithium-ion battery electrolytes: Building a platform and proof of principle studies. Chemical Engineering Journal, 2023, 455, 140955.	6.6	1
364	Artificial intelligence and machine learning in energy systems: A bibliographic perspective. Energy Strategy Reviews, 2023, 45, 101017.	3.3	44
365	How machine learning can accelerate electrocatalysis discovery and optimization. Materials Horizons, 2023, 10, 393-406.	6.4	24
366	A semi-automated material exploration scheme to predict the solubilities of tetraphenylporphyrin derivatives. Communications Chemistry, 2022, 5, .	2.0	2

#	ARTICLE	IF	CITATIONS
367	Graph neural networks for materials science and chemistry. <i>Communications Materials</i> , 2022, 3, .	2.9	90
368	Enhanced Cycle Stability of Low-Cost Na-Rich Metallic NaCl Electrode for Advanced Na-Ion Batteries. <i>Advanced Functional Materials</i> , 0, , 2210370.	7.8	0
369	Temperature- and Ambient Pressure-Independent Sensing of Hydrogen in Fluids Using Cascaded Interferometers Incorporated in Optical Fibers. <i>Advanced Materials Technologies</i> , 2023, 8, .	3.0	4
370	Engineering Single Atom Catalysts for Flow Production: From Catalyst Design to Reactor Understandings. <i>Accounts of Materials Research</i> , 2023, 4, 27-41.	5.9	7
371	Artificial Intelligence-Based Rapid Design of Grease with Chemically Functionalized Graphene and Carbon Nanotubes as Lubrication Additives. <i>Langmuir</i> , 2023, 39, 647-658.	1.6	7
372	A critical review on machine-learning-assisted screening and design of effective sorbents for carbon dioxide (CO <sub>2</sub> ) capture. <i>Frontiers in Energy Research</i> , 0, 10, .	1.2	2
373	Machine learning-assisted materials development and device management in batteries and supercapacitors: performance comparison and challenges. <i>Journal of Materials Chemistry A</i> , 2023, 11, 3904-3936.	5.2	5
374	Vending-Machine-Style Skin Excretion Sensing. <i>ACS Sensors</i> , 2023, 8, 326-334.	4.0	4
375	Earth-abundant photoelectrodes for water splitting and alternate oxidation reactions: Recent advances and future perspectives. <i>Progress in Materials Science</i> , 2023, 134, 101073.	16.0	15
376	Machine learning-based discovery of vibrationally stable materials. <i>Npj Computational Materials</i> , 2023, 9, .	3.5	3
377	Adaptive learning-driven high-throughput synthesis of oxygen reduction reaction Fe-N-C electrocatalysts. <i>Journal of Power Sources</i> , 2023, 559, 232583.	4.0	4
378	Robotic Powder Grinding with a Soft Jig for Laboratory Automation in Material Science. , 2022, , .		3
379	The rise of self-driving labs in chemical and materials sciences. , 2023, 2, 483-492.		63
380	Knowledge-integrated machine learning for materials: lessons from gaming and robotics. <i>Nature Reviews Materials</i> , 2023, 8, 241-260.	23.3	33
381	Using concentration gradients to examine the effects of Al, Ga and Sn additions on the low-activation VCrMnFe system. <i>JPhys Energy</i> , 2023, 5, 024013.	2.3	0
382	Recent Advances in Thermoregulatory Clothing: Materials, Mechanisms, and Perspectives. <i>ACS Nano</i> , 2023, 17, 1803-1830.	7.3	46
383	Predicting the HOMO-LUMO gap of benzenoid polycyclic hydrocarbons via interpretable machine learning. <i>Chemical Physics Letters</i> , 2023, 814, 140358.	1.2	6
384	Relationships between synthesis conditions and TiN coating properties discovered from the data driven approach. <i>Thin Solid Films</i> , 2023, 768, 139725.	0.8	5

#	ARTICLE	IF	CITATIONS
385	Data-driven designs and multi-scale simulations of enhanced ion transport in low-temperature operation for lithium-ion batteries. Korean Journal of Chemical Engineering, 2023, 40, 539-547.	1.2	3
386	Molecular Design Method based on New Molecular Representation and Variational Auto-encoder. , 2023, , .		1
387	Mathematical nuances of Gaussian process-driven autonomous experimentation. MRS Bulletin, 2023, 48, 153-163.	1.7	5
388	A robotic platform for the synthesis of colloidal nanocrystals. , 2023, 2, 505-514.		32
389	Deep transfer learning for predicting frontier orbital energies of organic materials using small data and its application to porphyrin photocatalysts. Physical Chemistry Chemical Physics, 2023, 25, 10536-10549.	1.3	4
390	Deep learning metal complex properties with natural quantum graphs. , 2023, 2, 618-633.		6
391	On the Importance of Fresh Stock Solutions for Surfactant-Free Colloidal Syntheses of Gold Nanoparticles in Alkaline Alcohol and Water Mixtures. Inorganics, 2023, 11, 140.	1.2	0
392	Autonomous experimental systems in materials science. Science and Technology of Advanced Materials Methods, 2023, 3, .	0.4	2
393	Artificial Intelligence in Material Engineering: A Review on Applications of Artificial Intelligence in Material Engineering. Advanced Engineering Materials, 2023, 25, .	1.6	5
394	Generative Models as an Emerging Paradigm in the Chemical Sciences. Journal of the American Chemical Society, 2023, 145, 8736-8750.	6.6	36
395	Recent advances and challenges of anodes for aqueous alkaline batteries. EnergyChem, 2023, 5, 100102.	10.1	2
396	Failure analysis of fiberglass cover used for photovoltaic plants. Journal of Applied Polymer Science, 2023, 140, .	1.3	2
407	Machine Learning Enabled Performance Prediction of Biomass-Derived Electrodes for Asymmetric Supercapacitor. Lecture Notes in Electrical Engineering, 2023, , 453-460.	0.3	0
411	The Surprising Ease of Finding Optimal Solutions for Controlling Nonlinear Phenomena in Quantum and Classical Complex Systems. Journal of Physical Chemistry A, 2023, 127, 4224-4236.	1.1	0
415	Discovery of Novel Photocatalysts Using Machine Learning Approach. , 2023, , 233-261.		0
424	Prediction of product distribution using machine learning techniques. Computer Aided Chemical Engineering, 2023, , 673-678.	0.3	0
426	A survey on advanced machine learning and deep learning techniques assisting in renewable energy generation. Environmental Science and Pollution Research, 2023, 30, 93407-93421.	2.7	0
439	Which Deep Learning Framework Should I Use: A Comparative Study For Deep Regression Modeling. , 2022, , .		0

#	ARTICLE	IF	CITATIONS
447	Accelerating the prediction of stable materials with machine learning. Nature Computational Science, 2023, 3, 934-945.	3.8	1
448	Realizing the cooking recipe of materials synthesis through large language models. Journal of Materials Chemistry A, 2023, 11, 25849-25853.	5.2	0
457	Accelerated Chemical Science with AI. , 0, , .		0
458	Robotic Powder Grinding with Audio-Visual Feedback for Laboratory Automation in Materials Science. , 2023, , .		0
470	Artificial intelligence in catalysis. , 2024, , 167-204.		0
472	Sustainable moisture energy. Nature Reviews Materials, 0, , .	23.3	0