Emerging materials intelligence ecosystems propelled b

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Citation Report

#	Article	IF	Citations
1	Machine learning for materials design and discovery. Journal of Applied Physics, 2021, 129, .	2.5	41
2	Efficient sampling for decision making in materials discovery*. Chinese Physics B, 2021, 30, 050705.	1.4	4
3	Autonomous Construction of Phase Diagrams of Block Copolymers by Theory-Assisted Active Machine Learning. ACS Macro Letters, 2021, 10, 598-602.	4.8	19
4	Big data and machine learning for materials science. Discover Materials, 2021, 1, 12.	2.8	49
5	Polymer informatics with multi-task learning. Patterns, 2021, 2, 100238.	5.9	43
6	Novel high voltage polymer insulators using computational and data-driven techniques. Journal of Chemical Physics, 2021, 154, 174906.	3.0	12
7	An Informatics Approach for Designing Conducting Polymers. ACS Applied Materials & Interfaces, 2021, 13, 53314-53322.	8.0	11
8	Predicting Polymersâ€™ Glass Transition Temperature by a Chemical Language Processing Model. Polymers, 2021, 13, 1898.	4.5	37
9	Copolymer Informatics with Multitask Deep Neural Networks. Macromolecules, 2021, 54, 5957-5961.	4.8	34
10	Machine learning in materials science: From explainable predictions to autonomous design. Computational Materials Science, 2021, 193, 110360.	3.0	103
11	Benchmarking graph neural networks for materials chemistry. Npj Computational Materials, 2021, 7, .	8.7	113
12	Learning with Delayed Rewardsâ€”A Case Study on Inverse Defect Design in 2D Materials. ACS Applied Materials & Interfaces, 2021, 13, 36455-36464.	8.0	12
13	Harnessing autocatalytic reactions in polymerization and depolymerization. MRS Communications, 2021, 11, 377-390.	1.8	4
14	Machine learning for alloys. Nature Reviews Materials, 2021, 6, 730-755.	48.7	202
15	Deep learning for visualization and novelty detection in large X-ray diffraction datasets. Npj Computational Materials, 2021, 7, .	8.7	28
16	polyG2G: A Novel Machine Learning Algorithm Applied to the Generative Design of Polymer Dielectrics. Chemistry of Materials, 2021, 33, 7008-7016.	6.7	23
17	Applying Machine Learning to Rechargeable Batteries: From the Microscale to the Macroscale. Angewandte Chemie - International Edition, 2021, 60, 24354-24366.	13.8	67
18	Machine-learning interatomic potentials for materials science. Acta Materialia, 2021, 214, 116980.	7.9	112

#	Article	IF	Citations
19	Applying Machine Learning to Rechargeable Batteries: From the Microscale to the Macroscale. Angewandte Chemie, 2021, 133, 24558-24570.	2.0	11
20	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	47.7	384
21	Machine learning on neutron and x-ray scattering and spectroscopies. Chemical Physics Reviews, 2021, 2, .	5.7	49
22	Design of polymers for energy storage capacitors using machine learning and evolutionary algorithms. Journal of Materials Science, 2021, 56, 19623-19635.	3.7	9
23	Machine learning assisted empirical formula augmentation. Materials and Design, 2021, 210, 110037.	7.0	8
24	Artificial intelligence and machine learning in design of mechanical materials. Materials Horizons, 2021, 8, 1153-1172.	12.2	237
25	Innovative Materials Science via Machine Learning. Advanced Functional Materials, 2022, 32, 2108044.	14.9	67
26	Computational Screening of MOFs and Zeolites for Direct Air Capture of Carbon Dioxide under Humid Conditions. Journal of Physical Chemistry C, 2021, 125, 24630-24639.	3.1	30
27	Construction of a machine-learning-based prediction model for mechanical properties of ultra-fine-grained Feâ€“C alloy. Journal of Materials Research and Technology, 2021, 15, 4914-4930.	5.8	13
28	Machine-Guided Polymer Knowledge Extraction Using Natural Language Processing: The Example of Named Entity Normalization. Journal of Chemical Information and Modeling, 2021, 61, 5377-5385.	5.4	9
29	Progress in Materials Data Availability and Application: A review. IEEE Signal Processing Magazine, 2022, 39, 104-108.	5.6	0
30	Learning in continuous action space for developing high dimensional potential energy models. Nature Communications, 2022, 13, 368.	12.8	21
31	Machine Learning and Natural Language Processing Enable a Data-Oriented Experimental Design Approach for Producing Biochar and Hydrochar from Biomass. Chemistry of Materials, 2022, 34, 979-990.	6.7	28
32	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. Chemistry of Materials, 2022, 34, 562-573.	6.7	8
33	Integration of Machine Learning and Coarse-Grained Molecular Simulations for Polymer Materials: Physical Understandings and Molecular Design. Frontiers in Chemistry, 2021, 9, 820417.	3.6	17
34	Advancing pharmacy and healthcare with virtual digital technologies. Advanced Drug Delivery Reviews, 2022, 182, 114098.	13.7	45
35	Machine Learning-Enabled Prediction and High-Throughput Screening of Polymer Membranes for Pervaporation Separation. ACS Applied Materials & Interfaces, 2022, 14, 8427-8436.	8.0	22
36	Photoelectrochemical Properties, Machine Learning, and Symbolic Regression for Molecularly Engineered Halide Perovskite Materials in Water. ACS Applied Materials & Interfaces, 2022, 14, 9933-9943.	8.0	12

#	Article	IF	Citations
37	Machine Learningâ€“Assisted Design of Material Properties. Annual Review of Chemical and Biomolecular Engineering, 2022, 13, 235-254.	6.8	13
38	Evaluation of performance of machine learning methods in mining structureâ€“property data of halide perovskite materials. Chinese Physics B, 2022, 31, 056302.	1.4	8
39	On the mechanics of shear deformable micro beams under thermo-mechanical loads using finite element analysis and deep learning neural network. Mechanics Based Design of Structures and Machines, 2023, 51, 6612-6656.	4.7	6
40	ARTS: autonomous research topic selection system using word embeddings and network analysis. Machine Learning: Science and Technology, 0, , .	5.0	2
41	Simple descriptor based machine learning model development for synergy prediction of different metal loadings and solvent swellings on coal pyrolysis. Chemical Engineering Science, 2022, 252, 117538.	3.8	7
42	Vision for energy material design: A roadmap for integrated data-driven modeling. Journal of Energy Chemistry, 2022, 71, 56-62.	12.9	12
43	Launching a materials informatics initiative for industrial applications in materials science, chemistry, and engineering. Pure and Applied Chemistry, 2022, 94, 637-642.	1.9	3
44	Inverse design of two-dimensional materials with invertible neural networks. Npj Computational Materials, 2021, 7, .	8.7	15
45	Incorporating Flexibility Effects into Metalâ€“Organic Framework Adsorption Simulations Using Different Models. ACS Applied Materials & Interfaces, 2021, 13, 61305-61315.	8.0	17
46	Formula Graph Selfâ€Attention Network for Representationâ€Domain Independent Materials Discovery. Advanced Science, 2022, 9, e2200164.	11.2	9
47	Materials Data toward Machine Learning: Advances and Challenges. Journal of Physical Chemistry Letters, 2022, 13, 3965-3977.	4.6	12
48	Conductivity prediction model for ionic liquids using machine learning. Journal of Chemical Physics, 2022, 156, .	3.0	8
49	Machine learning enabling high-throughput and remote operations at large-scale user facilities. , 2022, 1, 413-426.		10
50	Prediction of Phase Diagrams and Associated Phase Structural Properties. Industrial & Engineering Chemistry Research, 2022, 61, 8378-8389.	3.7	3
51	3D-structure-attention graph neural network for crystals and materials. Molecular Physics, 0, , .	1.7	1
52	Machine learning in concrete science: applications, challenges, and best practices. Npj Computational Materials, 2022, 8, .	8.7	79
53	Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. Chemical Reviews, 2022, 122, 13478-13515.	47.7	120
54	Deep neural networks based predictive-generative framework with data augmentation for designing composite materials. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 075003.	2.0	3

#	Article	IF	Citations
55	Machine Learning: A New Paradigm in Computational Electrocatalysis. Journal of Physical Chemistry Letters, 2022, 13, 7920-7930.	4.6	42
56	Artificial Intelligenceâ€Based Material Discovery for Clean Energy Future. Advanced Intelligent Systems, 2022, 4, .	6.1	9
57	Bayesian deep-learning for RUL prediction: An active learning perspective. Reliability Engineering and System Safety, 2022, 228, 108758.	8.9	34
58	Bayesian transfer learning with active querying for intelligent cross-machine fault prognosis under limited data. Mechanical Systems and Signal Processing, 2023, 183, 109628.	8.0	43
59	High-throughput informed machine learning models for ultrastrong B-N solids. Computational Materials Science, 2022, 215, 111789.	3.0	3
60	In silico active learning for small molecule properties. Molecular Systems Design and Engineering, 2022, 7, 1611-1621.	3.4	7
61	Machine learning of phase diagrams. Materials Advances, 0, , .	5.4	0
63	Machine Learning for Battery Research. SSRN Electronic Journal, 0, , .	0.4	0
64	Construction and Application of Music Style Intelligent Learning System Based on Situational Awareness. Mathematical Problems in Engineering, 2022, 2022, 1-11.	1.1	0
65	Estimation of the Flory-Huggins interaction parameter of polymer-solvent mixtures using machine learning. MRS Communications, 2022, 12, 1096-1102.	1.8	13
66	Rational design of all-organic flexible high-temperature polymer dielectrics. Matter, 2022, 5, 2615-2623.	10.0	21
67	Perspective on optimal strategies of building cluster expansion models for configurationally disordered materials. Journal of Chemical Physics, 2022, 157, .	3.0	4
68	Machine learning for battery research. Journal of Power Sources, 2022, 549, 232125.	7.8	22
69	Solvent selection for polymers enabled by generalized chemical fingerprinting and machine learning. Physical Chemistry Chemical Physics, 2022, 24, 26547-26555.	2.8	10
70	Machine learning overcomes human bias in the discovery of self-assembling peptides. Nature Chemistry, 2022, 14, 1427-1435.	13.6	36
71	Deep learning for electron and scanning probe microscopy: From materials design to atomic fabrication. MRS Bulletin, 2022, 47, 931-939.	3.5	14
72	Computational discovery of Metalâ€“Organic Frameworks for sustainable energy systems: Open challenges. Computers and Chemical Engineering, 2022, 167, 108022.	3.8	1
73	Bandgap model using symbolic regression for environmentally compatible lead-free inorganic double perovskites. , 2022, , .		0

#	Article	IF	Citations
74	Atomic structure generation from reconstructing structural fingerprints. Machine Learning: Science and Technology, 2022, 3, 045018.	5.0	3
75	Benchmarking AutoML for regression tasks on small tabular data in materials design. Scientific Reports, 2022, 12, .	3.3	10
76	Navigating the â€œKessel Runâ€•of digital materials acceleration. Patterns, 2022, 3, 100638.	5.9	0
77	Predicting Dielectric Polymer Component from Different Properties via Machine Learning Method. , 2022, , .		0
78	Predicting Dielectric Polymer Component from Different Properties via Machine Learning Method. , 2022, , .		0
79	Artificial Intelligence and Advanced Materials. Advanced Materials, 2023, 35, .	21.0	10
80	Bioplastic design using multitask deep neural networks. Communications Materials, 2022, 3, .	6.9	11
81	Machine Learning Potential Model Based on Ensemble Bispectrum Feature Selection and Its Applicability Analysis. Metals, 2023, 13, 169.	2.3	2
82	Emerging Trends in Machine Learning: A Polymer Perspective. ACS Polymers Au, 2023, 3, 239-258.	4.1	25
83	Exploring Explicit Coarse-Grained Structure in Artificial Neural Networks. Chinese Physics Letters, 2023, 40, 020501.	3.3	1
84	Machineâ€Learningâ€Assisted Nanozyme Design: Lessons from Materials and Engineered Enzymes. Advanced Materials, 2024, 36, .	21.0	14
85	Neuromorphic Computing for Scientific Applications. , 2022, , .		1
86	Constructing Microstructural Evolution System for Cement Hydration From Observed Data Using Deep Learning. IEEE Transactions on Systems, Man, and Cybernetics: Systems, 2023, 53, 4576-4589.	9.3	4
87	Polymer Informatics at Scale with Multitask Graph Neural Networks. Chemistry of Materials, 2023, 35, 1560-1567.	6.7	9
88	A Combined Data Science and Simulation-Based Methodology for Efficient and Economic Prediction of Thermoplastic Performance for Automotive Industry. , 0, , .		0
89	Deep learning-accelerated computational framework based on Physics Informed Neural Network for the solution of linear elasticity. Neural Networks, 2023, 162, 472-489.	5.9	19
90	Enhancing the bandwidth of antennas using polymer composites with high dielectric relaxation. , 2023, 3, 100026.		4
91	A data-driven physics-constrained deep learning computational framework for solving von Mises plasticity. Engineering Applications of Artificial Intelligence, 2023, 122, 106049.	8.1	17

#	Article	IF	Citations
92	Enhancing property prediction and process optimization in building materials through machine learning: A review. Computational Materials Science, 2023, 220, 112031.	3.0	20
93	Overview on Theoretical Simulations of Lithiumâ€ion Batteries and Their Application to Battery Separators. Advanced Energy Materials, 2023, 13, .	19.5	29
94	Discovery of thermosetting polymers with low hygroscopicity, low thermal expansivity, and high modulus by machine learning. Journal of Materials Chemistry A, 2023, 11, 12918-12927.	10.3	1
95	Drastic mass transport enhancement from miniscule precession. Matter, 2023, 6, 658-660.	10.0	0
96	Hybrid interatomic potential for Sn. Physical Review Materials, 2023, 7, .	2.4	2
97	Advances in machine learning- and artificial intelligence-assisted material design of steels. International Journal of Minerals, Metallurgy and Materials, 2023, 30, 1003-1024.	4.9	14
98	CoSMoR: Decoding decision-making process along continuous composition pathways in machine learning models trained for material properties. Physical Review Materials, 2023, 7, .	2.4	1
99	Decoding structure-spectrum relationships with physically organized latent spaces. Physical Review Materials, 2023, 7, .	2.4	4
100	Artificial-intelligence-led revolution of construction materials: From molecules to Industry 4.0. Matter, 2023, 6, 1831-1859.	10.0	13
101	Deep Learning in Mechanical Metamaterials: From Prediction and Generation to Inverse Design. Advanced Materials, 2023, 35, .	21.0	7
102	High-Throughput Screening and Prediction of High Modulus of Resilience Polymers Using Explainable Machine Learning. Journal of Chemical Theory and Computation, 2023, 19, 4641-4653.	5.3	2
103	Potential of Machine Learning Algorithms in Material Science: Predictions in Design, Properties, and Applications of Novel Functional Materials. , 2023, , 75-94.		0
104	High-Throughput in Situ Characterization of Polymer Crystallization under an Intense Flow, High Pressure, and Cooling Gradient during Injection Molding. Macromolecules, 2023, 56, 4111-4122.	4.8	5
105	polyBERT: a chemical language model to enable fully machine-driven ultrafast polymer informatics. Nature Communications, 2023, 14, .	12.8	16
107	Multi-reward reinforcement learning based development of inter-atomic potential models for silica. Npj Computational Materials, 2023, 9, .	8.7	1
108	AlphaMat: a material informatics hub connecting data, features, models and applications. Npj Computational Materials, 2023, 9, .	8.7	3
109	Exception Search in Databases for Polymers with Practically Contradictory Properties of Heat Resistance and Transparency. Polymer Chemistry, 0, , .	3.9	0
110	Machine learning assisted chemical characterization to investigate the temperature-dependent supercapacitance using Co-rGO electrodes. Carbon, 2023, 214, 118342.	10.3	0

#	Article	IF	Citations
111	The state of Augmented Reality in aerospace navigation and engineering. , 0, , .		0
112	A polymer genome approach for rational design of poly(aryl ether)s with high glass transition temperature. Journal of Materials Chemistry A, 2023, 11, 16985-16994.	10.3	1
113	Communicating Supraparticles to Enable Perceptual, Informationâ€Providing Matter. Advanced Materials, 2023, 35, .	21.0	1
114	Alloy synthesis and processing by semi-supervised text mining. Npj Computational Materials, 2023, 9, .	8.7	0
115	Physics-supervised deep learningâ€“based optimization (PSDLO) with accuracy and efficiency. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	1
117	Perspective: Machine Learning in Design for 3D/4D Printing. Journal of Applied Mechanics, Transactions ASME, 2024, 91, .	2.2	2
118	Few-shot ICD coding with knowledge transfer and evidence representation. Expert Systems With Applications, 2024, 238, 121861.	7.6	0
119	MatGPT: A Vane of Materials Informatics from Past, Present, to Future. Advanced Materials, 2024, 36, .	21.0	1
120	Evaluating Stage Motion for Automated Electron Microscopy. Microscopy and Microanalysis, 0, , .	0.4	1
121	Natural Products Derived Porous Carbons for CO₂ Capture. Advanced Science, 2023, 10, .	11.2	0
122	Machine learning and robot-assisted synthesis of diverse gold nanorods via seedless approach. , 2023, 1, 100028.		0
123	Examining graph neural networks for crystal structures: Limitations and opportunities for capturing periodicity. Science Advances, 2023, 9, .	10.3	1
124	Theory and Practice of Constructing College Physical Education Curricula Based on Immersive Multimedia Technology. International Journal of Web-Based Learning and Teaching Technologies, 2023, 18, 1-15.	0.9	0
126	Artificial intelligence-powered electronic skin. Nature Machine Intelligence, 2023, 5, 1344-1355.	16.0	4
128	Role of multifidelity data in sequential active learning materials discovery campaigns: case study of electronic bandgap. Machine Learning: Science and Technology, 2023, 4, 045060.	5.0	0
129	Interpretable scientific discovery with symbolic regression: a review. Artificial Intelligence Review, 2024, 57, .	15.7	0
130	Traditional or adaptive design of experiments? A pilot-scale comparison on wood delignification. Heliyon, 2024, 10, e24484.	3.2	0
131	Artificial intelligence (AI) enhanced finite element multiscale modeling and structural uncertainty analysis of a functionally graded porous beam. , 2024, , 251-269.		0

#	Article	IF	Citations
132	Machine Learning in Soft Matter: From Simulations to Experiments. Advanced Functional Materials, 0, , .	14.9	0
133	Blockchain-Based Security Access Control System for Sharing Squeeze Casting Process Database. Integrating Materials and Manufacturing Innovation, 2024, 13, 92-104.	2.6	0
134	Machine Learning Design for High-Entropy Alloys: Models and Algorithms. Metals, 2024, 14, 235.	2.3	0
135	Informatics-Driven Design of Superhard Bâ€“Câ€“O Compounds. ACS Applied Materials & Interfaces, 2024, 16, 10372-10379.	8.0	0
136	Network topology mapping of chemical compounds space. Scientific Reports, 2024, 14, .	3.3	0
137	Trends and Challenges in AIoT Implementation for Smart Home, Smart Buildings, and Smart Cities in Cloud Platforms. Advances in Computational Intelligence and Robotics Book Series, 2024, , 240-319.	0.4	0
138	Methods and applications of machine learning in computational design of optoelectronic semiconductors. Science China Materials, 2024, 67, 1042-1081.	6.3	0