

# Perspective: Materials informatics and big data: Realization of materials science in materials science

APL Materials

4, 053208

DOI: [10.1063/1.4946894](https://doi.org/10.1063/1.4946894)

Citation Report

#	ARTICLE	IF	CITATIONS
1	A Formation Energy Predictor for Crystalline Materials Using Ensemble Data Mining. , 2016, , .		14
2	Materials discovery: Understanding polycrystals from large-scale electron patterns. , 2016, , .		17
3	Preface: Special Topic on Materials Genome. APL Materials, 2016, 4, 053001.	2.2	9
4	MMOY: Towards deriving a metallic materials ontology from Yago. Advanced Engineering Informatics, 2016, 30, 687-702.	4.0	15
5	Predictive analytics for crystalline materials: bulk modulus. RSC Advances, 2016, 6, 95246-95251.	1.7	62
6	A general-purpose machine learning framework for predicting properties of inorganic materials. Npj Computational Materials, 2016, 2, .	3.5	922
7	Understanding and designing magnetoelectric heterostructures guided by computation: progresses, remaining questions, and perspectives. Npj Computational Materials, 2017, 3, .	3.5	110
8	Accessing Materials Data: Challenges and Directions in the Digital Era. Integrating Materials and Manufacturing Innovation, 2017, 6, 172-186.	1.2	6
9	High-throughput DFT calculations of formation energy, stability and oxygen vacancy formation energy of ABO <sub>3</sub> perovskites. Scientific Data, 2017, 4, 170153.	2.4	259
10	Hierarchical nanoporous metals as a path toward the ultimate three-dimensional functionality. Science and Technology of Advanced Materials, 2017, 18, 724-740.	2.8	50
11	Designing Nanostructures for Phonon Transport via Bayesian Optimization. Physical Review X, 2017, 7, .	2.8	127
12	Elucidating multi-physics interactions in suspensions for the design of polymeric dispersants: a hierarchical machine learning approach. Molecular Systems Design and Engineering, 2017, 2, 263-273.	1.7	26
13	Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations. Physical Review B, 2017, 96, .	1.1	254
14	Materials discovery and design using machine learning. Journal of Materiomics, 2017, 3, 159-177.	2.8	629
15	Towards a Hybrid Human-Computer Scientific Information Extraction Pipeline. , 2017, , .		18
16	From properties to materials: An efficient and simple approach. Journal of Chemical Physics, 2017, 147, 234105.	1.2	16
17	Materials Science Literature-Patent Relevance Search: A Heterogeneous Network Analysis Approach. , 2017, , .		2
18	How to make decisions with algorithms. ORBIT Journal, 2017, 1, 1-13.	0.9	0

#	ARTICLE	IF	CITATIONS
19	Data Sampling Schemes for Microstructure Design with Vibrational Tuning Constraints. <i>AIAA Journal</i> , 2018, 56, 1239-1250.	1.5	9
20	Data Mining for Parameters Affecting Polymorph Selection in Contorted Hexabenzocoronene Derivatives. <i>Chemistry of Materials</i> , 2018, 30, 3330-3337.	3.2	9
21	Composition design for (PrNd <sup>2</sup> La <sup>2</sup> Ce) <sub>2</sub> Fe <sub>14</sub> B melt-spun magnets by machine learning technique. <i>Chinese Physics B</i> , 2018, 27, 047501.	0.7	1
22	Representing molecular and materials data for unsupervised machine learning. <i>Molecular Simulation</i> , 2018, 44, 905-920.	0.9	18
23	Materials Informatics. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1313-1314.	2.5	4
24	A Systematic Machine Learning Based Approach for the Diagnosis of Non-Alcoholic Fatty Liver Disease Risk and Progression. <i>Scientific Reports</i> , 2018, 8, 2112.	1.6	56
25	Computational microstructure characterization and reconstruction: Review of the state-of-the-art techniques. <i>Progress in Materials Science</i> , 2018, 95, 1-41.	16.0	252
26	Adaptive design of an X-ray magnetic circular dichroism spectroscopy experiment with Gaussian process modelling. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	38
27	Machine learning properties of binary wurtzite superlattices. <i>Journal of Materials Science</i> , 2018, 53, 6652-6664.	1.7	24
28	Materials 4.0: Materials big data enabled materials discovery. <i>Applied Materials Today</i> , 2018, 10, 127-132.	2.3	118
29	Recognizing Local and Global Structural Motifs at the Atomic Scale. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 486-498.	2.3	43
30	Prediction of seebeck coefficient for compounds without restriction to fixed stoichiometry: A machine learning approach. <i>Journal of Computational Chemistry</i> , 2018, 39, 191-202.	1.5	65
31	Texture based image classification for nanoparticle surface characterisation and machine learning. <i>JPhys Materials</i> , 2018, 1, 016001.	1.8	5
32	Towards Simulation-Data Science – A Case Study on Material Failures. , 2018, , .		0
33	A Deep Adversarial Learning Methodology for Designing Microstructural Material Systems. , 2018, , .		27
34	Machine Learning-Based Reduce Order Crystal Plasticity Modeling for ICME Applications. <i>Integrating Materials and Manufacturing Innovation</i> , 2018, 7, 214-230.	1.2	36
35	ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition. <i>Scientific Reports</i> , 2018, 8, 17593.	1.6	242
36	Multi-Information Source Fusion and Optimization to Realize ICME: Application to Dual-Phase Materials. <i>Journal of Mechanical Design, Transactions of the ASME</i> , 2018, 140, .	1.7	32

#	ARTICLE	IF	CITATIONS
37	How to make decisions with algorithms. <i>ACM SIGCAS Computers and Society</i> , 2018, 47, 122-133.	0.1	4
38	Combinatorial approaches for the design of metallic alloys. <i>Comptes Rendus Physique</i> , 2018, 19, 737-754.	0.3	29
39	Improved adaptive sampling method utilizing Gaussian process regression for prediction of spectral peak structures. <i>Applied Physics Express</i> , 2018, 11, 112401.	1.1	20
40	Important Descriptors and Descriptor Groups of Curie Temperatures of Rare-earth Transition-metal Binary Alloys. <i>Journal of the Physical Society of Japan</i> , 2018, 87, 113801.	0.7	26
41	Chances and Challenges in Fusing Data Science with Materials Science. <i>Praktische Metallographie/Practical Metallography</i> , 2018, 55, 493-514.	0.1	8
42	Extracting Grain Orientations from EBSD Patterns of Polycrystalline Materials Using Convolutional Neural Networks. <i>Microscopy and Microanalysis</i> , 2018, 24, 497-502.	0.2	46
43	Identifying an efficient, thermally robust inorganic phosphor host via machine learning. <i>Nature Communications</i> , 2018, 9, 4377.	5.8	228
44	Big Semantic Data Processing in the Materials Design Domain. , 2018, , 1-8.		2
45	Predicting Thermodynamic Properties of Alkanes by High-Throughput Force Field Simulation and Machine Learning. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2502-2516.	2.5	23
46	Polar projections for big data analysis in applied superconductivity. <i>AIP Advances</i> , 2018, 8, .	0.6	7
47	Microstructural Materials Design Via Deep Adversarial Learning Methodology. <i>Journal of Mechanical Design, Transactions of the ASME</i> , 2018, 140, .	1.7	142
48	Perspectives on the Impact of Machine Learning, Deep Learning, and Artificial Intelligence on Materials, Processes, and Structures Engineering. <i>Integrating Materials and Manufacturing Innovation</i> , 2018, 7, 157-172.	1.2	205
49	Data-Driven Materials Investigations: The Next Frontier in Understanding and Predicting Fatigue Behavior. <i>Jom</i> , 2018, 70, 1143-1146.	0.9	22
50	Deep learning approaches for mining structure-property linkages in high contrast composites from simulation datasets. <i>Computational Materials Science</i> , 2018, 151, 278-287.	1.4	219
51	A strategy to apply machine learning to small datasets in materials science. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	404
52	Spectroscopic Studies on the Metal-Insulator Transition Mechanism in Correlated Materials. <i>Advanced Materials</i> , 2018, 30, e1704777.	11.1	18
53	Learning atoms for materials discovery. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E6411-E6417.	3.3	138
54	Bioinspired hierarchical composite design using machine learning: simulation, additive manufacturing, and experiment. <i>Materials Horizons</i> , 2018, 5, 939-945.	6.4	354

#	ARTICLE	IF	CITATIONS
55	Deep Learning in Data-Driven Pavement Image Analysis and Automated Distress Detection: A Review. <i>Data</i> , 2018, 3, 28.	1.2	106
56	Machine learning for molecular and materials science. <i>Nature</i> , 2018, 559, 547-555.	13.7	2,387
57	Machine learning modeling of superconducting critical temperature. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	274
58	Computer-Aided Screening of Conjugated Polymers for Organic Solar Cell: Classification by Random Forest. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2639-2646.	2.1	135
59	Deep Semi-supervised Learning for Virtual Screening Based on Big Data Analytics. <i>Communications in Computer and Information Science</i> , 2018, , 173-184.	0.4	1
60	Predicting the effective thermal conductivities of composite materials and porous media by machine learning methods. <i>International Journal of Heat and Mass Transfer</i> , 2018, 127, 908-916.	2.5	187
61	The 2019 materials by design roadmap. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 013001.	1.3	236
62	Innovative Data Management in advanced characterization: Implications for materials design. <i>Materials Today Communications</i> , 2019, 20, 100541.	0.9	20
63	Prediction and optimization of mechanical properties of composites using convolutional neural networks. <i>Composite Structures</i> , 2019, 227, 111264.	3.1	118
64	IRNet. , 2019, , .		23
65	Prediction of repeat unit of optimal polymer by Bayesian optimization. <i>MRS Advances</i> , 2019, 4, 1125-1130.	0.5	9
66	Nanoinformatics, and the big challenges for the science of small things. <i>Nanoscale</i> , 2019, 11, 19190-19201.	2.8	59
67	Data-driven discovery of formulas by symbolic regression. <i>MRS Bulletin</i> , 2019, 44, 559-564.	1.7	48
68	Predicting the onset temperature ( $T_g$ ) of Ge Se $_{1-x}$ glass transition: a feature selection based two-stage support vector regression method. <i>Science Bulletin</i> , 2019, 64, 1195-1203.	4.3	41
69	A simple descriptor for binding and charge transfer at blue phosphorene-metal interfaces. <i>Applied Surface Science</i> , 2019, 492, 16-22.	3.1	5
70	Materials science in the artificial intelligence age: high-throughput library generation, machine learning, and a pathway from correlations to the underpinning physics. <i>MRS Communications</i> , 2019, 9, 821-838.	0.8	109
71	Deep materials informatics: Applications of deep learning in materials science. <i>MRS Communications</i> , 2019, 9, 779-792.	0.8	137
72	Materials data specification: Methods and use cases. <i>Computational Materials Science</i> , 2019, 169, 109086.	1.4	4

#	ARTICLE	IF	CITATIONS
73	Predicting Microstructure-Sensitive Fatigue-Crack Path in 3D Using a Machine Learning Framework. <i>Jom</i> , 2019, 71, 2680-2694.	0.9	41
74	Predicting the effective thermal conductivity of composites from cross sections images using deep learning methods. <i>Composites Science and Technology</i> , 2019, 184, 107861.	3.8	90
75	Data-Driven Materials Science: Status, Challenges, and Perspectives. <i>Advanced Science</i> , 2019, 6, 1900808.	5.6	358
76	Machine learning in materials science. <i>Informa-ÃnÃ-MateriÃjly</i> , 2019, 1, 338-358.	8.5	427
77	Deep learning based domain knowledge integration for small datasets: Illustrative applications in materials informatics. , 2019, , .		9
78	An Image Texture Descriptor based Machine Learning Framework for Prediction of Thermo-Mechanic Heat Treatment Process in Plain Carbon Steel. , 2019, , .		0
79	Machine-learning-assisted thin-film growth: Bayesian optimization in molecular beam epitaxy of SrRuO3 thin films. <i>APL Materials</i> , 2019, 7, .	2.2	55
80	Data science-enabled molecular-to-systems engineering for sustainable water treatment. <i>Current Opinion in Chemical Engineering</i> , 2019, 26, 122-130.	3.8	22
81	Visualizing Scientistsâ€™ Cognitive Representation of Materials Data through the Application of Ontology. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7482-7491.	2.1	16
82	Virtual Issue on Machine-Learning Discoveries in Materials Science. <i>Chemistry of Materials</i> , 2019, 31, 8243-8247.	3.2	23
83	Big Data Creates New Opportunities for Materials Research: A Review on Methods and Applications of Machine Learning for Materials Design. <i>Engineering</i> , 2019, 5, 1017-1026.	3.2	181
84	Ontological Concepts and Taxonomies for Nano World. <i>Journal of Information and Knowledge Management</i> , 2019, 18, 1950014.	0.8	2
85	Deep learning approach for segmentation of plain carbon steel microstructure images. <i>IET Image Processing</i> , 2019, 13, 1516-1524.	1.4	11
86	High-performance bifunctional polarization switch chiral metamaterials by inverse design method. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	33
87	Predicting Materials Properties with Little Data Using Shotgun Transfer Learning. <i>ACS Central Science</i> , 2019, 5, 1717-1730.	5.3	223
88	Predicting Twin Nucleation in a Polycrystalline Mg Alloy Using Machine Learning Methods. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2019, 50, 5543-5560.	1.1	23
89	Performance Prediction in Nuclear Materials by Using a Collaborative Framework of Supercomputing, Big Data and Artificial Intelligence. <i>Communications in Computer and Information Science</i> , 2019, , 97-110.	0.4	0
90	Automated generation of carbon nanotube morphology in cement composite via data-driven approaches. <i>Composites Part B: Engineering</i> , 2019, 167, 51-62.	5.9	20

#	ARTICLE	IF	CITATIONS
91	Viscoelasticity of Short Polymer Liquids from Atomistic Simulations. Journal of the Electrochemical Society, 2019, 166, B3246-B3256.	1.3	19
92	Completing the picture through correlative characterization. Nature Materials, 2019, 18, 1041-1049.	13.3	73
93	An acceleration search method of higher $T_c$ superconductors by a machine learning algorithm. Applied Physics Express, 2019, 12, 073003.	1.1	31
94	Materials Informatics Approach to the Identification of One-Band Correlated Materials Analogous to the Cuprates. Physical Review X, 2019, 9, .	2.8	4
95	Exploring effective charge in electromigration using machine learning. MRS Communications, 2019, 9, 567-575.	0.8	18
96	Identifying hidden high-dimensional structure/property relationships using self-organizing maps. MRS Communications, 2019, 9, 730-736.	0.8	3
97	Monte Carlo tree search for materials design and discovery. MRS Communications, 2019, 9, 532-536.	0.8	34
98	Molecular Engineering of Superplasticizers for Metakaolin-Portland Cement Blends with Hierarchical Machine Learning. Advanced Theory and Simulations, 2019, 2, 1800164.	1.3	20
99	Using artificial intelligence to accelerate materials development. MRS Bulletin, 2019, 44, 335-344.	1.7	16
100	Materials Discovery and Properties Prediction in Thermal Transport via Materials Informatics: A Mini Review. Nano Letters, 2019, 19, 3387-3395.	4.5	94
101	Hierarchical Machine Learning Model for Mechanical Property Predictions of Polyurethane Elastomers From Small Datasets. Frontiers in Materials, 2019, 6, .	1.2	18
102	MatCALO: Knowledge-enabled machine learning in materials science. Computational Materials Science, 2019, 163, 50-62.	1.4	25
103	Multifidelity Information Fusion with Machine Learning: A Case Study of Dopant Formation Energies in Hafnia. ACS Applied Materials & Interfaces, 2019, 11, 24906-24918.	4.0	49
104	Classifying and predicting the electron affinity of diamond nanoparticles using machine learning. Nanoscale Horizons, 2019, 4, 983-990.	4.1	15
105	Multisize and multiweight effects in materials science and engineering. Science China Technological Sciences, 2019, 62, 707-710.	2.0	17
106	Data mining new energy materials from structure databases. Renewable and Sustainable Energy Reviews, 2019, 107, 554-567.	8.2	38
107	Physics-Guided Data-Mining Driven Design of Room-Temperature Multiferroic Perovskite Oxides. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900028.	1.2	2
108	Knowledge discovery through chemical space networks: the case of organic electronics. Journal of Molecular Modeling, 2019, 25, 87.	0.8	14

#	ARTICLE	IF	CITATIONS
109	Data-enabled structure-property mappings for lanthanide-activated inorganic scintillators. <i>Journal of Materials Science</i> , 2019, 54, 8361-8380.	1.7	9
110	Identifying Pb-free perovskites for solar cells by machine learning. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	129
111	Heteroanionic Materials by Design: Progress Toward Targeted Properties. <i>Advanced Materials</i> , 2019, 31, e1805295.	11.1	150
112	Systems Approaches to Materials Design: Past, Present, and Future. <i>Annual Review of Materials Research</i> , 2019, 49, 103-126.	4.3	49
113	Progress toward autonomous experimental systems for alloy development. <i>MRS Bulletin</i> , 2019, 44, 273-280.	1.7	32
114	Automated estimation of materials parameter from X-ray absorption and electron energy-loss spectra with similarity measures. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	37
115	Visualising multi-dimensional structure/property relationships with machine learning. <i>JPhys Materials</i> , 2019, 2, 034003.	1.8	20
116	Materials Informatics for Heat Transfer: Recent Progresses and Perspectives. <i>Nanoscale and Microscale Thermophysical Engineering</i> , 2019, 23, 157-172.	1.4	41
117	Bandgap prediction by deep learning in configurationally hybridized graphene and boron nitride. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	86
118	From DFT to machine learning: recent approaches to materials science—a review. <i>JPhys Materials</i> , 2019, 2, 032001.	1.8	385
119	Rich multi-dimensional correlative imaging. <i>IOP Conference Series: Materials Science and Engineering</i> , 2019, 580, 012014.	0.3	4
120	Incomplete Conditional Density Estimation for Fast Materials Discovery. , 2019, , 549-557.		2
121	Martensite Start Temperature Predictor for Steels Using Ensemble Data Mining. , 2019, , .		4
122	Ontology-based methods of thermophysical data integration. <i>Journal of Physics: Conference Series</i> , 2019, 1385, 012033.	0.3	2
123	Data-Driven Insights from Predictive Analytics on Heterogeneous Experimental Data of Industrial Magnetic Materials. , 2019, , .		2
124	Transfer Learning Using Ensemble Neural Networks for Organic Solar Cell Screening. , 2019, , .		11
125	Estimating Regions of Deterioration in Electron Microscope Images of Rubber Materials via a Transfer Learning-Based Anomaly Detection Model. <i>IEEE Access</i> , 2019, 7, 162395-162404.	2.6	4
126	Predicting structure/property relationships in multi-dimensional nanoparticle data using t-distributed stochastic neighbour embedding and machine learning. <i>Nanoscale</i> , 2019, 11, 23165-23172.	2.8	24



#	ARTICLE	IF	CITATIONS
127	Enhancing materials property prediction by leveraging computational and experimental data using deep transfer learning. <i>Nature Communications</i> , 2019, 10, 5316.	5.8	160
128	Selecting Doping Elements by Data Mining for Advanced Magnets. <i>Chemistry of Materials</i> , 2019, 31, 10117-10125.	3.2	12
129	Prediction of Absorption Spectrum Shifts in Dyes Adsorbed on Titania. <i>Scientific Reports</i> , 2019, 9, 16983.	1.6	27
130	Representing Multiword Chemical Terms through Phrase-Level Preprocessing and Word Embedding. <i>ACS Omega</i> , 2019, 4, 18510-18519.	1.6	7
131	Mapping intrinsic electromechanical responses at the nanoscale via sequential excitation scanning probe microscopy empowered by deep data. <i>National Science Review</i> , 2019, 6, 55-63.	4.6	27
132	The Rise of Catalyst Informatics: Towards Catalyst Genomics. <i>ChemCatChem</i> , 2019, 11, 1146-1152.	1.8	72
133	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2019, , 1-28.		6
134	Establishing structure-property localization linkages for elastic deformation of three-dimensional high contrast composites using deep learning approaches. <i>Acta Materialia</i> , 2019, 166, 335-345.	3.8	125
135	Soft Matter Informatics: Current Progress and Challenges. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800129.	1.3	52
136	Data-driven evaluation of fatigue performance of additive manufactured parts using miniature specimens. <i>Journal of Materials Science and Technology</i> , 2019, 35, 1137-1146.	5.6	59
137	Finding the Right Bricks for Molecular Legos: A Data Mining Approach to Organic Semiconductor Design. <i>Chemistry of Materials</i> , 2019, 31, 969-978.	3.2	38
138	Automatic estimation of mechanical properties from fractographs using optimal anisotropic diffusion and Voronoi tessellation. <i>Measurement: Journal of the International Measurement Confederation</i> , 2019, 134, 574-585.	2.5	6
139	An automated algorithm for reliable equation of state fitting of magnetic systems. <i>Computational Materials Science</i> , 2019, 156, 121-128.	1.4	2
140	Accelerating high-throughput searches for new alloys with active learning of interatomic potentials. <i>Computational Materials Science</i> , 2019, 156, 148-156.	1.4	218
141	Materials informatics. <i>Journal of Intelligent Manufacturing</i> , 2019, 30, 2307-2326.	4.4	90
142	Simulation and design of energy materials accelerated by machine learning. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1421.	6.2	41
143	A high throughput molecular screening for organic electronics via machine learning: present status and perspective. <i>Japanese Journal of Applied Physics</i> , 2020, 59, SD0801.	0.8	43
144	Predicting degradation rate of genipin cross-linked gelatin scaffolds with machine learning. <i>Materials Science and Engineering C</i> , 2020, 107, 110362.	3.8	21

#	ARTICLE	IF	CITATIONS
145	Materials knowledge reasoning with production based system. Computational Materials Science, 2020, 173, 109317.	1.4	0
146	High-Throughput Experimentation and Catalyst Informatics for Oxidative Coupling of Methane. ACS Catalysis, 2020, 10, 921-932.	5.5	117
147	Learning acoustic emission signatures from a nanoindentation-based lithography process: Towards rapid microstructure characterization. Tribology International, 2020, 143, 106074.	3.0	14
148	Using Deep Machine Learning to Understand the Physical Performance Bottlenecks in Novel Thin-Film Solar Cells. Advanced Functional Materials, 2020, 30, 1907259.	7.8	36
149	Mining materials knowledge with concept lattice algorithm. Materials Today Communications, 2020, 22, 100726.	0.9	2
150	Coupling in situ experiments and modeling – Opportunities for data fusion, machine learning, and discovery of emergent behavior. Current Opinion in Solid State and Materials Science, 2020, 24, 100797.	5.6	21
151	Predicting the effects of microstructure on matrix crack initiation in fiber reinforced ceramic matrix composites via machine learning. Composite Structures, 2020, 236, 111702.	3.1	26
152	Crystallographic prediction from diffraction and chemistry data for higher throughput classification using machine learning. Computational Materials Science, 2020, 173, 109409.	1.4	27
153	Invited review: Machine learning for materials developments in metals additive manufacturing. Additive Manufacturing, 2020, 36, 101641.	1.7	61
154	Machine Learning-Based Evaluation of Shear Capacity of Recycled Aggregate Concrete Beams. Materials, 2020, 13, 4552.	1.3	24
155	The role of technological innovation in plastic production within a circular economy framework. Resources, Conservation and Recycling, 2020, 163, 105094.	5.3	44
156	Adaptive machine learning for efficient materials design. MRS Bulletin, 2020, 45, 579-586.	1.7	16
157	Scientific AI in materials science: a path to a sustainable and scalable paradigm. Machine Learning: Science and Technology, 2020, 1, 033001.	2.4	35
158	Machine learning-driven new material discovery. Nanoscale Advances, 2020, 2, 3115-3130.	2.2	111
159	Machine Learning for Electronically Excited States of Molecules. Chemical Reviews, 2021, 121, 9873-9926.	23.0	207
160	Designing thermal functional materials by coupling thermal transport calculations and machine learning. Journal of Applied Physics, 2020, 128, .	1.1	17
161	Autonomous materials synthesis by machine learning and robotics. APL Materials, 2020, 8, .	2.2	69
162	Machine Learning Prediction of Nine Molecular Properties Based on the SMILES Representation of the QM9 Quantum-Chemistry Dataset. Journal of Physical Chemistry A, 2020, 124, 9854-9866.	1.1	50

#	ARTICLE	IF	CITATIONS
163	Machine-learning predictions of polymer properties with Polymer Genome. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	111
164	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	181
165	Application of big data analytics and organizational performance: the mediating role of knowledge management practices. <i>Journal of Big Data</i> , 2020, 7, .	6.9	38
166	Halide Perovskite Materials for Energy Storage Applications. <i>Advanced Functional Materials</i> , 2020, 30, 2003653.	7.8	63
167	Prediction of the Bilinear Stress-Strain Curve of Aluminum Alloys Using Artificial Intelligence and Big Data. <i>Metals</i> , 2020, 10, 904.	1.0	16
168	A novel method to predict the stiffness evolution of in-service wind turbine blades based on deep learning models. <i>Composite Structures</i> , 2020, 252, 112702.	3.1	15
169	Machine-learning-assisted search for functional materials over extended chemical space. <i>Materials Horizons</i> , 2020, 7, 2710-2718.	6.4	14
170	An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	39
171	Data centric nanocomposites design <i>via</i> mixed-variable Bayesian optimization. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1376-1390.	1.7	15
172	Machine learning for accelerating the discovery of high-performance donor/acceptor pairs in non-fullerene organic solar cells. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	77
173	Benchmarking materials property prediction methods: the Matbench test set and Automatminer reference algorithm. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	96
174	Method construction of structure-property relationships from data by machine learning assisted mining for materials design applications. <i>Materials and Design</i> , 2020, 196, 109194.	3.3	24
175	Fuzzy Logic and Fuzzy Expert System-Based Material Synthesis Methods. , 0, , .		4
176	Predicting Tensile Properties of AZ31 Magnesium Alloys by Machine Learning. <i>Jom</i> , 2020, 72, 3935-3942.	0.9	30
177	Exploring the landscape of model representations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 24061-24068.	3.3	29
178	Designing and understanding light-harvesting devices with machine learning. <i>Nature Communications</i> , 2020, 11, 4587.	5.8	57
179	<i>In silico</i> investigation of Cu(In,Ga)Se <sub>2</sub> -based solar cells. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26682-26701.	1.3	3
180	Featureless adaptive optimization accelerates functional electronic materials design. <i>Applied Physics Reviews</i> , 2020, 7, .	5.5	26

#	ARTICLE	IF	CITATIONS
181	Variation in Mechanical Properties of Ti-13Nb-13Zr Depending on Annealing Temperature. Applied Sciences (Switzerland), 2020, 10, 7896.	1.3	8
182	Modeling of metal nanoparticles: Development of neural-network interatomic potential inspired by features of the modified embedded-atom method. Physical Review B, 2020, 102, .	1.1	3
183	Automated identification of deformation twin systems in Mg WE43 from SEM DIC. Materials Characterization, 2020, 169, 110628.	1.9	12
184	Machine Learning for Structural Materials. Annual Review of Materials Research, 2020, 50, 27-48.	4.3	29
185	Machine learning in materials genome initiative: A review. Journal of Materials Science and Technology, 2020, 57, 113-122.	5.6	110
186	Learning physical properties of liquid crystals with deep convolutional neural networks. Scientific Reports, 2020, 10, 7664.	1.6	44
187	Metal 3D printing as a disruptive technology for superalloys. Nature Communications, 2020, 11, 2327.	5.8	159
188	Understanding the ML black box with simple descriptors to predict cluster adsorbate interaction energy. New Journal of Chemistry, 2020, 44, 8545-8553.	1.4	7
189	Topology optimization of 2D structures with nonlinearities using deep learning. Computers and Structures, 2020, 237, 106283.	2.4	108
190	Accelerating Development of Materials for Industrial and High-Tech Applications with Data-Driven Analysis and Simulations. MRS Advances, 2020, 5, 1497-1511.	0.5	0
191	High-throughput determination of high-quality interdiffusion coefficients in metallic solids: a review. Journal of Materials Science, 2020, 55, 10303-10338.	1.7	34
192	Towards systems tissue engineering: Elucidating the dynamics, spatial coordination, and individual cells driving emergent behaviors. Biomaterials, 2020, 255, 120189.	5.7	8
193	Opportunities and Challenges for Machine Learning in Materials Science. Annual Review of Materials Research, 2020, 50, 71-103.	4.3	183
194	Machine-Learning-Optimized Aperiodic Superlattice Minimizes Coherent Phonon Heat Conduction. Physical Review X, 2020, 10, .	2.8	61
195	Machine learning of mechanical properties of steels. Science China Technological Sciences, 2020, 63, 1247-1255.	2.0	70
196	Synergy of Binary Substitutions for Improving the Cycle Performance in LiNiO <sub>2</sub> Revealed by Ab Initio Materials Informatics. ACS Omega, 2020, 5, 13403-13408.	1.6	8
197	A novel gradient composition spreading and nanolayer stacking process for combinatorial thin-film materials library fabrication. Review of Scientific Instruments, 2020, 91, 065107.	0.6	5
198	Discovery and design of soft polymeric bio-inspired materials with multiscale simulations and artificial intelligence. Journal of Materials Chemistry B, 2020, 8, 6562-6587.	2.9	44

#	ARTICLE	IF	CITATIONS
199	Prediction of optoelectronic properties of Cu <sub>2</sub> O using neural network potential. Physical Chemistry Chemical Physics, 2020, 22, 14910-14917.	1.3	2
200	Big-data driven approaches in materials science: A survey. Materials Today: Proceedings, 2020, 26, 1245-1249.	0.9	10
201	The covalent radii derived from the first-principle data. Molecular Physics, 2020, 118, e1742937.	0.8	2
202	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100
203	Quantitative structure–property relationship of the photoelectrochemical oxidation of phenolic pollutants at modified nanoporous titanium oxide using supervised machine learning. Physical Chemistry Chemical Physics, 2020, 22, 8878-8888.	1.3	10
204	A review of mathematical representations of biomolecular data. Physical Chemistry Chemical Physics, 2020, 22, 4343-4367.	1.3	56
205	Machine learning assisted materials design and discovery for rechargeable batteries. Energy Storage Materials, 2020, 31, 434-450.	9.5	212
206	Pavement Image Datasets: A New Benchmark Dataset to Classify and Densify Pavement Distresses. Transportation Research Record, 2020, 2674, 328-339.	1.0	94
207	A Design-to-Device Pipeline for Data-Driven Materials Discovery. Accounts of Chemical Research, 2020, 53, 599-610.	7.6	59
208	An Efficient Approach to Consolidating Job Schedulers in Traditional Independent Scientific Workflows. Applied Sciences (Switzerland), 2020, 10, 1455.	1.3	2
209	Genetic algorithm-driven discovery of unexpected thermal conductivity enhancement by disorder. Nano Energy, 2020, 71, 104619.	8.2	57
210	Artificial Intelligence to Power the Future of Materials Science and Engineering. Advanced Intelligent Systems, 2020, 2, 1900143.	3.3	75
211	Critical Temperature Prediction of Superconductors Based on Atomic Vectors and Deep Learning. Symmetry, 2020, 12, 262.	1.1	19
212	Machine learning: Accelerating materials development for energy storage and conversion. Informa <i>Analytics</i> -Materials, 2020, 2, 553-576.	8.5	212
213	Feature Engineering of Solid-State Crystalline Lattices for Machine Learning. Advanced Theory and Simulations, 2020, 3, 1900190.	1.3	3
214	Computational functionality-driven design of semiconductors for optoelectronic applications. Informa <i>Analytics</i> -Materials, 2020, 2, 879-904.	8.5	32
215	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. Polymers, 2020, 12, 163.	2.0	95
216	Carbon science perspective in 2020: Current research and future challenges. Carbon, 2020, 161, 373-391.	5.4	77

#	ARTICLE	IF	CITATIONS
217	A Computational Approach to the Microstructural Design of High-Speed Steels. <i>Steel Research International</i> , 2020, 91, 1900455.	1.0	2
218	Electron microscopy characterization of fast reactor MOX Joint Oxyde-Gaine (JOG). <i>Journal of Nuclear Materials</i> , 2020, 531, 151964.	1.3	13
219	The Materials Simulation Toolkit for Machine learning (MAST-ML): An automated open source toolkit to accelerate data-driven materials research. <i>Computational Materials Science</i> , 2020, 176, 109544.	1.4	42
220	Computational Prediction of Critical Temperatures of Superconductors Based on Convolutional Gradient Boosting Decision Trees. <i>IEEE Access</i> , 2020, 8, 57868-57878.	2.6	17
221	Deep machine learning approach to develop a new asphalt pavement condition index. <i>Construction and Building Materials</i> , 2020, 247, 118513.	3.2	139
222	Nanomaterial Synthesis Insights from Machine Learning of Scientific Articles by Extracting, Structuring, and Visualizing Knowledge. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2876-2887.	2.5	35
223	Recent progress on discovery and properties prediction of energy materials: Simple machine learning meets complex quantum chemistry. <i>Journal of Energy Chemistry</i> , 2021, 54, 72-88.	7.1	32
224	Analytic formulas of peak current in cyclic voltammogram: Machine learning as an alternative way?. <i>Journal of Chemometrics</i> , 2021, 35, e3314.	0.7	10
225	Modeling the chemo-mechanical behavior of all-solid-state batteries: a review.. <i>Meccanica</i> , 2021, 56, 1523-1554.	1.2	41
226	ALKEMIE: An intelligent computational platform for accelerating materials discovery and design. <i>Computational Materials Science</i> , 2021, 186, 110064.	1.4	89
227	Artificial Intelligence in Materials Modeling and Design. <i>Archives of Computational Methods in Engineering</i> , 2021, 28, 3399-3413.	6.0	34
228	Two-dimensional Janus material MoS <sub>2</sub> (1-x)Se <sub>2x</sub> (0 ≤ x ≤ 1) for photovoltaic applications: A machine learning and density functional study. <i>Computational Materials Science</i> , 2021, 186, 109998.	1.4	9
229	Artificial intelligence in nuclear industry: Chimera or solution?. <i>Journal of Cleaner Production</i> , 2021, 278, 124022.	4.6	35
230	Machine learning (ML)-assisted optimization doping of KI in MAPbI <sub>3</sub> solar cells. <i>Rare Metals</i> , 2021, 40, 1698-1707.	3.6	21
231	Tailoring nanoprecipitates for ultra-strong high-entropy alloys via machine learning and prestrain aging. <i>Journal of Materials Science and Technology</i> , 2021, 69, 156-167.	5.6	48
232	Machine learning in experimental materials chemistry. <i>Catalysis Today</i> , 2021, 371, 77-84.	2.2	36
233	Solving Stochastic Inverse Problems for Property-Structure Linkages Using Data-Consistent Inversion and Machine Learning. <i>Jom</i> , 2021, 73, 72-89.	0.9	16
234	How Machine Learning Accelerates the Development of Quantum Dots. <i>Chinese Journal of Chemistry</i> , 2021, 39, 181-188.	2.6	10

#	ARTICLE	IF	CITATIONS
235	Buckling and postbuckling of architected materials: A review of methods for lattice structures and metal foams. <i>Composites and Advanced Materials</i> , 2021, 30, 263498332110039.	0.5	2
236	Nanofiber Extracellular Matrices in Regenerative Medicine. <i>Fundamental Biomedical Technologies</i> , 2021, , 235-251.	0.2	0
237	Accelerated Development of High-Strength Magnesium Alloys by Machine Learning. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2021, 52, 943-954.	1.1	18
238	Thermal Nanostructure Design by Materials Informatics. <i>Springer Series in Materials Science</i> , 2021, , 153-195.	0.4	0
239	Enabling deeper learning on big data for materials informatics applications. <i>Scientific Reports</i> , 2021, 11, 4244.	1.6	29
240	How the Shape of Chemical Data Can Enable Data-Driven Materials Discovery. <i>Trends in Chemistry</i> , 2021, 3, 111-119.	4.4	9
241	EXPLORATORY DATA ANALYSIS ON MACROSCOPIC MATERIAL BEHAVIOR USING MICROMECHANICAL SIMULATIONS BY APPLYING THE GAUSSIAN PROCESSES WITH VARIOUS KERNELS. <i>Indian Journal of Computer Science and Engineering</i> , 2021, 12, 246-253.	0.2	1
242	Exploring Heat-Shielding Nanoparticle-Based Materials via First-Principles Calculations and Transfer Learning. <i>ACS Applied Nano Materials</i> , 2021, 4, 1932-1939.	2.4	2
243	Transferable Multilevel Attention Neural Network for Accurate Prediction of Quantum Chemistry Properties via Multitask Learning. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1066-1082.	2.5	63
244	Chemist versus Machine: Traditional Knowledge versus Machine Learning Techniques. <i>Trends in Chemistry</i> , 2021, 3, 86-95.	4.4	36
245	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. <i>Trends in Chemistry</i> , 2021, 3, 96-110.	4.4	39
246	Combinatorial Screening of Cuprate Superconductors by Drop-On-Demand Inkjet Printing. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 9101-9112.	4.0	13
247	Machine learning approach for the prediction and optimization of thermal transport properties. <i>Frontiers of Physics</i> , 2021, 16, 1.	2.4	39
248	Optimization of the composition in a composite material for microelectronics application using the Ising model. <i>Scientific Reports</i> , 2021, 11, 3057.	1.6	5
249	Machine learning for material characterization with an application for predicting mechanical properties. <i>GAMM Mitteilungen</i> , 2021, 44, e202100003.	2.7	32
250	Correlation-Based Framework for Extraction of Insights from Quantum Chemistry Databases: Applications for Nanoclusters. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1125-1135.	2.5	3
251	ChemProps: A RESTful API enabled database for composite polymer name standardization. <i>Journal of Cheminformatics</i> , 2021, 13, 22.	2.8	7
252	High-throughput screening and machine learning for the efficient growth of high-quality single-wall carbon nanotubes. <i>Nano Research</i> , 2021, 14, 4610-4615.	5.8	11



#	ARTICLE	IF	CITATIONS
253	Linking knowledge management capabilities and the mediating role of the big data capabilities for enterprise value-adding processes. VINE Journal of Information and Knowledge Management Systems, 2023, 53, 64-79.	1.2	3
254	Self-Driving Laboratories for Development of New Functional Materials and Optimizing Known Reactions. Nanomaterials, 2021, 11, 619.	1.9	28
255	Clustering Algorithms: An Application for Adsorption Kinetic Curves. IEEE Latin America Transactions, 2021, 19, 507-514.	1.2	1
256	Machine learning autonomous identification of magnetic alloys beyond the Slater-Pauling limit. Communications Materials, 2021, 2, .	2.9	25
257	Machine Learning for Transition-Metal-Based Hydrogen Generation Electrocatalysts. ACS Catalysis, 2021, 11, 3930-3937.	5.5	38
258	A contemporary approach to the MSE paradigm powered by Artificial Intelligence from a review focused on Polymer Matrix Composites. Mechanics of Advanced Materials and Structures, 2022, 29, 3076-3096.	1.5	9
259	Learning interpretable descriptors for the fatigue strength of steels. AIP Advances, 2021, 11, .	0.6	4
260	Materials discovery through machine learning formation energy. JPhys Energy, 2021, 3, 022002.	2.3	36
261	Machine learning approaches for permittivity prediction and rational design of microwave dielectric ceramics. Journal of Materiomics, 2021, 7, 1284-1293.	2.8	16
262	A microstructure-informatic strategy for Vickers hardness forecast of austenitic steels from experimental data. Materials and Design, 2021, 201, 109497.	3.3	11
263	Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. Journal of Physics Condensed Matter, 2021, 33, 194006.	0.7	7
264	Biased decision making in materials science: Where does it originate and can it be avoided?. MRS Bulletin, 2021, 46, 361-367.	1.7	2
265	Modeling processâ€“structureâ€“property relationships in metal additive manufacturing: a review on physics-driven versus data-driven approaches. JPhys Materials, 2021, 4, 032002.	1.8	46
266	Machine learning augmented predictive and generative model for rupture life in ferritic and austenitic steels. Npj Materials Degradation, 2021, 5, .	2.6	23
267	Compositionally restricted attention-based network for materials property predictions. Npj Computational Materials, 2021, 7, .	3.5	68
268	Study on Prediction of Compression Performance of Composite Laminates After Impact Based on Convolutional Neural Networks. Applied Composite Materials, 2021, 28, 1153-1173.	1.3	9
269	Agricultural and rural ecological management system based on big data in complex system. Environmental Technology and Innovation, 2021, 22, 101390.	3.0	8
270	A Review of Application of Machine Learning in Design, Synthesis, and Characterization of Metal Matrix Composites: Current Status and Emerging Applications. Jom, 2021, 73, 2060-2074.	0.9	24



#	ARTICLE	IF	CITATIONS
271	A physics-informed machine learning approach for solving heat transfer equation in advanced manufacturing and engineering applications. <i>Engineering Applications of Artificial Intelligence</i> , 2021, 101, 104232.	4.3	144
272	Predicting Single-Substance Phase Diagrams: A Kernel Approach on Graph Representations of Molecules. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4488-4497.	1.1	7
273	Machine learning approaches for feature engineering of the crystal structure: Application to the prediction of the formation energy of cubic compounds. <i>Physical Review Materials</i> , 2021, 5, .	0.9	6
274	Efficient hyperparameter tuning for kernel ridge regression with Bayesian optimization. <i>Machine Learning: Science and Technology</i> , 2021, 2, 035022.	2.4	28
275	Experimental Investigations of Micro-Meso Damage Evolution for a Co/WC-Type Tool Material with Application of Digital Image Correlation and Machine Learning. <i>Materials</i> , 2021, 14, 3562.	1.3	8
276	Encoding the atomic structure for machine learning in materials science. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, e1558.	6.2	29
277	Prediction of chemical compounds properties using a deep learning model. <i>Neural Computing and Applications</i> , 2021, 33, 13345-13366.	3.2	18
278	Porous Metal Properties Analysis: A Machine Learning Approach. <i>Jom</i> , 2021, 73, 2039-2049.	0.9	3
279	Mechanical behavior predictions of additively manufactured microstructures using functional Gaussian process surrogates. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	14
280	High-Throughput Evaluation of Discharge Profiles of Nickel Substitution in LiNiO <sub>2</sub> by Ab Initio Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 14517-14524.	1.5	5
281	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. <i>Chemical Reviews</i> , 2021, 121, 9816-9872.	23.0	287
282	Application of deep transfer learning to predicting crystal structures of inorganic substances. <i>Computational Materials Science</i> , 2021, 195, 110476.	1.4	11
283	Innovative and Economically Beneficial Use of Corn and Corn Products in Electrochemical Energy Storage Applications. <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 10678-10703.	3.2	9
284	Impact of the Characteristics of Quantum Chemical Databases on Machine Learning Prediction of Tautomerization Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4769-4785.	2.3	12
285	Teaching solid mechanics to artificial intelligence—a fast solver for heterogeneous materials. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	55
286	Robust model benchmarking and bias-imbalance in data-driven materials science: a case study on MODNet. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 404002.	0.7	12
287	A deep learning based life prediction method for components under creep, fatigue and creep-fatigue conditions. <i>International Journal of Fatigue</i> , 2021, 148, 106236.	2.8	99
288	The data-intensive scientific revolution occurring where two-dimensional materials meet machine learning. <i>Cell Reports Physical Science</i> , 2021, 2, 100482.	2.8	26

#	ARTICLE	IF	CITATIONS
289	Catalyze Materials Science with Machine Learning. , 2021, 3, 1151-1171.		28
290	Emergence of machine learning in the development of high entropy alloy and their prospects in advanced engineering applications. Emergent Materials, 2021, 4, 1635-1648.	3.2	21
291	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	23.0	110
292	Data-Driven Approaches Toward Smarter Additive Manufacturing. Advanced Intelligent Systems, 2021, 3, 2100014.	3.3	21
293	A machine-learning approach to predict creep properties of Cr-Mo steel with time-temperature parameters. Journal of Materials Research and Technology, 2021, 13, 635-650.	2.6	41
294	Computational Design of Dielectric Materials: Background and Perspectives. Journal of the Institute of Electrical Engineers of Japan, 2021, 141, 516-519.	0.0	0
295	Automated stopping criterion for spectral measurements with active learning. Npj Computational Materials, 2021, 7, .	3.5	17
296	Convolutional neural network model for synchrotron radiation imaging datasets to automatically detect interfacial microstructure: An in situ process monitoring tool during solar PV ribbon fabrication. Solar Energy, 2021, 224, 230-244.	2.9	6
297	Crystal-Site-Based Artificial Neural Networks for Material Classification. Crystals, 2021, 11, 1039.	1.0	3
298	Machine learning workflow for microparticle composite thin-film process-structure linkages. Journal of Coatings Technology Research, 2022, 19, 83-96.	1.2	3
299	Stochastic characterization and reconstruction of material microstructures for establishment of process-structure-property linkage using the deep generative model. Physical Review E, 2021, 104, 025302.	0.8	25
300	Reliability evaluation method for squeeze casting process parameter data. International Journal of Advanced Manufacturing Technology, 2021, 117, 1303.	1.5	1
301	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
302	A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling. Journal of Chemical Education, 2021, 98, 2892-2898.	1.1	41
303	Hystorian: A processing tool for scanning probe microscopy and other n-dimensional datasets. Ultramicroscopy, 2021, 228, 113345.	0.8	3
304	Machine learning-based prediction of supercapacitor performance for a novel electrode material: Cerium oxynitride. Energy Storage Materials, 2021, 40, 426-438.	9.5	35
305	Estimating the mechanical residual strength from IR spectra using machine learning for degraded adhesives. Journal of Adhesion, 2022, 98, 2423-2445.	1.8	8
306	Adoption of Image-Driven Machine Learning for Microstructure Characterization and Materials Design: A Perspective. Jom, 2021, 73, 3639-3657.	0.9	6

#	ARTICLE	IF	CITATIONS
307	Machine Learning: An Advanced Platform for Materials Development and State Prediction in Lithium-Ion Batteries. <i>Advanced Materials</i> , 2022, 34, e2101474.	11.1	140
308	Development of surrogate predictive models for the nonlinear elasto-plastic response of medium density fibreboard-based sandwich structures. <i>International Journal of Lightweight Materials and Manufacture</i> , 2021, 4, 302-314.	1.3	4
309	Machine learning-based discovery of molecules, crystals, and composites: A perspective review. <i>Korean Journal of Chemical Engineering</i> , 2021, 38, 1971-1982.	1.2	4
310	Materials Fingerprinting Classification. <i>Computer Physics Communications</i> , 2021, 266, 108019.	3.0	6
311	Feature Blending: An Approach toward Generalized Machine Learning Models for Property Prediction. <i>ACS Physical Chemistry Au</i> , 2022, 2, 16-22.	1.9	6
312	Uncertainty Quantification of Metallic Microstructures with Analytical and Machine Learning Based Approaches. <i>AIAA Journal</i> , 0, , 1-12.	1.5	2
313	Data-Driven Discovery of 2D Materials for Solar Water Splitting. <i>Frontiers in Materials</i> , 2021, 8, .	1.2	8
314	The machine-learned radii of atoms. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113389.	1.1	1
315	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. <i>Science Bulletin</i> , 2021, 66, 1973-1985.	4.3	32
316	Machine learning elastic constants of multi-component alloys. <i>Computational Materials Science</i> , 2021, 198, 110671.	1.4	36
317	Emerging artificial intelligence in piezoelectric and triboelectric nanogenerators. <i>Nano Energy</i> , 2021, 88, 106227.	8.2	76
318	Accurate prediction of high-temperature elastic constants of Ti <sub>0.5</sub> Al <sub>0.5</sub> N random alloy. <i>Thin Solid Films</i> , 2021, 735, 138872.	0.8	4
319	Additive manufacturability of superalloys: Process-induced porosity, cooling rate and metal vapour. <i>Additive Manufacturing</i> , 2021, 47, 102339.	1.7	3
320	Machine learning-based predictions of fatigue life and fatigue limit for steels. <i>Journal of Materials Science and Technology</i> , 2021, 90, 9-19.	5.6	68
321	Bayesian neural networks for uncertainty quantification in data-driven materials modeling. <i>Computer Methods in Applied Mechanics and Engineering</i> , 2021, 386, 114079.	3.4	44
322	Machine learning-enabled prediction of chemical durability of A <sub>2</sub> B <sub>2</sub> O <sub>7</sub> pyrochlore and fluorite. <i>Computational Materials Science</i> , 2021, 200, 110820.	1.4	11
323	Data Science, Machine Learning and Artificial Intelligence Applied to Metals and Alloys Research: Past, Present, and Future. , 2022, , 609-621.		2
324	Nonferrous waste aerated concrete. <i>Journal of Applied Engineering Science</i> , 2021, 19, 788-794.	0.4	0

#	ARTICLE	IF	CITATIONS
325	Uncertainty Quantification of the Metallic Microstructures with Analytical and Machine Learning Based Approaches. , 2021, , .		0
326	Machine learning for perovskite materials design and discovery. Npj Computational Materials, 2021, 7, .	3.5	189
327	Big Data-Driven Materials Science and Its FAIR Data Infrastructure. , 2019, , 1-25.		5
328	Big Data-Driven Materials Science and Its FAIR Data Infrastructure. , 2020, , 49-73.		18
329	CALYPSO Method for Structure Prediction and Its Applications to Materials Discovery. , 2020, , 2729-2756.		3
330	Microstructure optimization with constrained design objectives using machine learning-based feedback-aware data-generation. Computational Materials Science, 2019, 160, 334-351.	1.4	41
331	Deformation behavior and amorphization in icosahedral boron-rich ceramics. Progress in Materials Science, 2020, 112, 100664.	16.0	34
332	Modelling and understanding battery materials with machine-learning-driven atomistic simulations. JPhys Energy, 2020, 2, 041003.	2.3	51
333	Machine learning enabled discovery of application dependent design principles for two-dimensional materials. Machine Learning: Science and Technology, 2020, 1, 035015.	2.4	9
334	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. Physical Review Materials, 2018, 2, .	0.9	349
335	Autonomous efficient experiment design for materials discovery with Bayesian model averaging. Physical Review Materials, 2018, 2, .	0.9	58
336	CRYSPNet: Crystal structure predictions via neural networks. Physical Review Materials, 2020, 4, .	0.9	26
337	Strategic Key Elements in Big Data Analytics as Driving Forces of IoT Manufacturing Value Creation: A Challenge for Research Framework. IEEE Transactions on Engineering Management, 2024, 71, 90-105.	2.4	3
338	Predicting the thermodynamic stability of perovskite oxides using multiple machine learning techniques. Materials Today: Proceedings, 2022, 52, 457-461.	0.9	6
339	Photocatalytic Zâ€šScheme Overall Water Splitting: Recent Advances in Theory and Experiments. Advanced Materials, 2021, 33, e2105195.	11.1	123
340	Bioactive Synthetic Polymers. Advanced Materials, 2022, 34, e2105063.	11.1	66
341	Artificial intelligence for search and discovery of quantum materials. Communications Materials, 2021, 2, .	2.9	29
342	Innovative Materials Science via Machine Learning. Advanced Functional Materials, 2022, 32, 2108044.	7.8	67

#	ARTICLE	IF	CITATIONS
343	Data Science Applied to Carbon Materials: Synthesis, Characterization, and Applications. Advanced Theory and Simulations, 2022, 5, 2100205.	1.3	3
344	Rational Design of Polymer Dielectrics: An Application of Density Functional Theory and Machine Learning. , 2018, , 293-319.		1
345	Big Semantic Data Processing in the Materials Design Domain. , 2019, , 358-365.		0
346	Prediction of Electropulse-Induced Nonlinear Temperature Variation of Mg Alloy Based on Machine Learning. Journal of Korean Institute of Metals and Materials, 2020, 58, 413-422.	0.4	10
347	A Machine Learning-based surrogate modeling framework for predicting the history-dependent deformation of dual phase microstructures. Materials Today Communications, 2021, 29, 102914.	0.9	5
348	Identification of Microstructures in 3-Dâ€“Printed Ti-6Al-4V Using Acoustic Emission Cepstrum. Smart and Sustainable Manufacturing Systems, 2020, 4, 163-178.	0.3	4
349	Die Materialsynthesemaschine. Nachrichten Aus Der Chemie, 2020, 68, 66-69.	0.0	1
350	Machine learning and materials informatics approaches in the analysis of physical properties of carbon nanotubes: A review. Computational Materials Science, 2022, 201, 110939.	1.4	41
351	A highly interpretable materials informatics approach for predicting microstructure-property relationship in fabric composites. Composites Science and Technology, 2022, 217, 109080.	3.8	15
352	Digital Transformation in Plastics Industry: From Digitization Toward Virtual Material. Future of Business and Finance, 2020, , 287-298.	0.3	0
353	Materials Image Informatics Using Deep Learning. , 2020, , 205-230.		2
354	Microstructure classification in the unsupervised context. Acta Materialia, 2022, 223, 117434.	3.8	10
355	Thermodynamic and electronic properties of ReN <sub>2</sub> polymorphs at high pressure. Physical Review B, 2021, 104, .	1.1	1
356	Determining liquid crystal properties with ordinal networks and machine learning. Chaos, Solitons and Fractals, 2022, 154, 111607.	2.5	19
357	Prediction of solar cell materials via unsupervised literature learning. Journal of Physics Condensed Matter, 2022, 34, 095902.	0.7	5
358	Uncertainty Prediction for Machine Learning Models of Material Properties. ACS Omega, 2021, 6, 32431-32440.	1.6	21
359	Data-driven thermoelectric modeling: Current challenges and prospects. Journal of Applied Physics, 2021, 130, .	1.1	9
360	Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data. Nature Communications, 2021, 12, 6595.	5.8	55

#	ARTICLE	IF	CITATIONS
361	Implications of the BATTERY 2030+ AI-Assisted Toolkit on Future Low-CO <sub>2</sub> Battery Discoveries and Chemistries. <i>Advanced Energy Materials</i> , 2022, 12, 2102698.	10.2	20
362	Prediction of stiffness degradation based on machine learning: Axial elastic modulus of [0m /90n ]s composite laminates. <i>Composites Science and Technology</i> , 2022, 218, 109186.	3.8	14
363	Statistical learning of small data with domain knowledge --- sample size- and pre-notch length-dependent strength of concrete. <i>Engineering Fracture Mechanics</i> , 2022, 259, 108160.	2.0	6
364	Computational modeling of green hydrogen generation from photocatalytic H <sub>2</sub> S splitting: Overview and perspectives. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2021, 49, 100456.	5.6	15
365	A hybrid PSO and Grey Wolf Optimization algorithm for static and dynamic crack identification. <i>Theoretical and Applied Fracture Mechanics</i> , 2022, 118, 103213.	2.1	58
366	Investigating the Impact of Synthetic Data Distribution on the Performance of Regression Models to Overcome Small Dataset Problems. , 2020, , .		2
367	Development of Materials Informatics Platform. <i>Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi]</i> , 2021, 34, 41-47.	0.1	3
368	Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis. <i>Topics in Catalysis</i> , 2022, 65, 6-39.	1.3	27
369	Imputation Method Based on Collaborative Filtering and Clustering for the Missing Data of the Squeeze Casting Process Parameters. <i>Integrating Materials and Manufacturing Innovation</i> , 2022, 11, 95-108.	1.2	3
370	Machine-learning and high-throughput studies for high-entropy materials. <i>Materials Science and Engineering Reports</i> , 2022, 147, 100645.	14.8	44
371	Global-Oriented Strategy for Searching Ultrastrength Martensitic Stainless Steels. <i>Advanced Theory and Simulations</i> , 0, , 2100411.	1.3	4
372	Deep-learning-based porous media microstructure quantitative characterization and reconstruction method. <i>Physical Review E</i> , 2022, 105, 015308.	0.8	18
373	Neural Network Potentials: A Concise Overview of Methods. <i>Annual Review of Physical Chemistry</i> , 2022, 73, 163-186.	4.8	69
374	Potential Application of Machine-Learning-Based Quantum Chemical Methods in Environmental Chemistry. <i>Environmental Science &amp; Technology</i> , 2022, 56, 2115-2123.	4.6	22
375	Fatigue modeling using neural networks: A comprehensive review. <i>Fatigue and Fracture of Engineering Materials and Structures</i> , 2022, 45, 945-979.	1.7	79
376	Predicting plastic anisotropy using crystal plasticity and Bayesian neural network surrogate models. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2022, 833, 142472.	2.6	6
377	The Potential of Machine Learning for Enhancing CO <sub>2</sub> Sequestration, Storage, Transportation, and Utilization-based Processes: A Brief Perspective. <i>Jom</i> , 2022, 74, 414-428.	0.9	24
378	Highly accurate machine learning prediction of crystal point groups for ternary materials from chemical formula. <i>Scientific Reports</i> , 2022, 12, 1577.	1.6	9

#	ARTICLE	IF	CITATIONS
379	Smart Materials Prediction: Applying Machine Learning to Lithium Solid-State Electrolyte. <i>Materials</i> , 2022, 15, 1157.	1.3	10
380	Machine learning approaches for prediction of properties of natural fiber composites : Apriori algorithm. <i>Australian Journal of Mechanical Engineering</i> , 0, , 1-16.	1.5	2
381	Recent trends in computational tools and data-driven modeling for advanced materials. <i>Materials Advances</i> , 2022, 3, 4069-4087.	2.6	17
382	Biomimicry for natural and synthetic composites and use of machine learning in hierarchical design. , 2022, , 141-182.		1
383	A Machine Learning Method for Material Property Prediction: Example Polymer Compatibility. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
384	Functional Nanomaterials Design in the Workflow of Building Machine-Learning Models. <i>Lecture Notes in Networks and Systems</i> , 2022, , 370-383.	0.5	0
385	Learning Matter: Materials Design with Machine Learning and Atomistic Simulations. <i>Accounts of Materials Research</i> , 2022, 3, 343-357.	5.9	31
386	Large scale dataset of real space electronic charge density of cubic inorganic materials from density functional theory (DFT) calculations. <i>Scientific Data</i> , 2022, 9, 59.	2.4	1
387	Role of the Backbone when Optimizing Functional Groupsâ€™â€™A Theoretical Study Based on an Improved Inverse-Design Approach. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1289-1299.	1.1	1
388	A review of the recent progress in battery informatics. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	53
389	Machine Learning-Assisted High-Throughput Virtual Screening for On-Demand Customization of Advanced Energetic Materials. <i>Engineering</i> , 2022, 10, 99-109.	3.2	18
390	Inverse Design of Materials by Machine Learning. <i>Materials</i> , 2022, 15, 1811.	1.3	28
391	Data Centric Design: A New Approach to Design of Microstructural Material Systems. <i>Engineering</i> , 2022, 10, 89-98.	3.2	18
392	Predicting Youngâ€™s Modulus of Linear Polyurethane and Polyurethaneâ€™â€™Polyurea Elastomers: Bridging Length Scales with Physicochemical Modeling and Machine Learning. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 16568-16581.	4.0	14
393	Collective Variables for Free Energy Surface Tailoring: Understanding and Modifying Functionality in Systems Dominated by Rare Events. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2830-2837.	2.1	5
394	Combinatorial synthesis of heteroepitaxial, multi-cation, thin-films via pulsed laser deposition coupled with in-situ, chemical and structural characterization. <i>Scientific Reports</i> , 2022, 12, 3219.	1.6	2
395	Many-Scale Investigations of the Deformation Behavior of Polycrystalline Composites: lâ€™Machine Learning Applied for Image Segmentation. <i>Materials</i> , 2022, 15, 2486.	1.3	1
396	Machine Learning for the Discovery, Design, and Engineering of Materials. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2022, 13, 405-429.	3.3	10



#	ARTICLE	IF	CITATIONS
397	Microtomographic Analysis of a Palaeolithic Wooden Point from the Ljubljana River. <i>Sensors</i> , 2022, 22, 2369.	2.1	1
398	Machine learning in energy storage materials. , 2022, 1, 175-195.		45
399	Emerging Strategies for CO <sub>2</sub> Photoreduction to CH <sub>4</sub> : From Experimental to Data-Driven Design. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	68
400	How Machine Learning Predicts and Explains the Performance of Perovskite Solar Cells. <i>Solar Rrl</i> , 2022, 6, .	3.1	26
401	Emerging Trends in Sustainable CO <sub>2</sub> Management Materials. <i>Advanced Materials</i> , 2022, 34, e2201547.	11.1	52
402	Data-driven design of soft sensors. <i>Nature Machine Intelligence</i> , 2022, 4, 194-195.	8.3	2
403	Current Trends in Fluid Research in the Era of Artificial Intelligence: A Review. <i>Fluids</i> , 2022, 7, 116.	0.8	27
404	Recent advances and applications of deep learning methods in materials science. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	207
405	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
406	Lattice inversion potential with neural network corrections for metallic systems. <i>Computational Materials Science</i> , 2022, 207, 111311.	1.4	1
407	Predicting glass properties by using physics- and chemistry-informed machine learning models. <i>Journal of Non-Crystalline Solids</i> , 2022, 584, 121511.	1.5	8
408	High throughput screening driven discovery of Mn <sub>5</sub> Co <sub>10</sub> Fe <sub>30</sub> Ni <sub>55</sub> O <sub>x</sub> as electrocatalyst for water oxidation and electrospinning synthesis. <i>Applied Surface Science</i> , 2022, 588, 152959.	3.1	6
409	Knowledge Graph-Empowered Materials Discovery. , 2021, , .		4
410	Towards Predictive Synthesis of Inorganic Materials Using Network Science. <i>Frontiers in Chemistry</i> , 2021, 9, 798838.	1.8	2
411	Inverse Design of Nanoparticles Using Multi-Target Machine Learning. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	18
412	Data-Driven Methods for Accelerating Polymer Design. <i>ACS Polymers Au</i> , 2022, 2, 8-26.	1.7	39
413	Accelerated HKUST-1 Thin-Film Property Optimization Using Active Learning. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 61827-61837.	4.0	4
414	Recent Progress and Future Prospects on All-Organic Polymer Dielectrics for Energy Storage Capacitors. <i>Chemical Reviews</i> , 2022, 122, 3820-3878.	23.0	240



#	ARTICLE	IF	CITATIONS
415	Molecular representations for machine learning applications in chemistry. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	26
416	Lossless multi-scale constitutive elastic relations with artificial intelligence. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	18
417	A Perspective on Digital Knowledge Representation in Materials Science and Engineering. <i>Advanced Engineering Materials</i> , 2022, 24, .	1.6	10
418	Learning the crystal structure genome for property classification. <i>Physical Review Research</i> , 2022, 4, .	1.3	2
419	Data-Driven Approach to Designing Two-dimensional Van der Waals Heterostructures: Misjudgment of Band Alignment Type and its mechanism. <i>Physica Status Solidi - Rapid Research Letters</i> , 0, , .	1.2	2
423	Tailoring Vibrational Signature and Functionality of 2D-Ordered Linear-Chain Carbon-Based Nanocarriers for Predictive Performance Enhancement of High-End Energetic Materials. <i>Nanomaterials</i> , 2022, 12, 1041.	1.9	2
424	Perspectives in the new era of materials intelligent design. , 0, 1, .		2
425	A Framework of the Value Co-Creation Cycle in Platform Businesses: An Exploratory Case Study. <i>Sustainability</i> , 2022, 14, 5612.	1.6	3
426	From materials discovery to system optimization by integrating combinatorial electrochemistry and data science. <i>Current Opinion in Electrochemistry</i> , 2022, 35, 101053.	2.5	17
427	Discovery of direct band gap perovskites for light harvesting by using machine learning. <i>Computational Materials Science</i> , 2022, 210, 111476.	1.4	18
428	Skill-Agnostic analysis of reflection high-energy electron diffraction patterns for Si(111) surface superstructures using machine learning. <i>Science and Technology of Advanced Materials Methods</i> , 2022, 2, 162-174.	0.4	6
429	Intrinsic physics in magnetic Weyl semimetal SrRuO <sub>3</sub> films addressed by machine-learning-assisted molecular beam epitaxy. <i>Japanese Journal of Applied Physics</i> , 2023, 62, SA0801.	0.8	6
430	Assessment of Outliers in Alloy Datasets Using Unsupervised Techniques. <i>Jom</i> , 2022, 74, 2846-2859.	0.9	3
431	Machine learning of fake micrographs for automated analysis of crystal growth process. <i>Science and Technology of Advanced Materials Methods</i> , 2022, 2, 213-221.	0.4	3
432	Recent Achievements in Experimental and Computational Studies of Positive Electrode Materials for Nonaqueous Ca- and Al-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 9209-9227.	1.5	5
433	Molecular Modeling in Anion Exchange Membrane Research: A Brief Review of Recent Applications. <i>Molecules</i> , 2022, 27, 3574.	1.7	6
435	Perovskite- and Dye-Sensitized Solar-Cell Device Databases Auto-generated Using ChemDataExtractor. <i>Scientific Data</i> , 2022, 9, .	2.4	24
436	Autonomous materials discovery and manufacturing (AMDM): A review and perspectives. <i>IISE Transactions</i> , 2023, 55, 75-93.	1.6	5

#	ARTICLE	IF	CITATIONS
437	Machine Learning Applications in Composites: Manufacturing, Design, and Characterization. ACS Symposium Series, 0, , 65-85.	0.5	0
438	Machine-learning exploration of polymer compatibility. Cell Reports Physical Science, 2022, 3, 100931.	2.8	15
439	Auto-generating databases of Yield Strength and Grain Size using ChemDataExtractor. Scientific Data, 2022, 9, .	2.4	13
440	Material machine learning for alloys: Applications, challenges and perspectives. Journal of Alloys and Compounds, 2022, 921, 165984.	2.8	39
441	Machine learning in concrete science: applications, challenges, and best practices. Npj Computational Materials, 2022, 8, .	3.5	79
442	Data in Materials and Catalysts Informatics. ACS Symposium Series, 0, , 239-246.	0.5	2
443	Design of silicon-containing arylacetylene resins aided by machine learning enhanced materials genome approach. Chemical Engineering Journal, 2022, 448, 137643.	6.6	17
444	Continually Reactivating Iterative-Projection Process Method for Instantiating Microstructure from Two-Point Statistics. SSRN Electronic Journal, 0, , .	0.4	0
446	Data-driven chemistry. , 2022, , 233-240.		0
447	Enhancing thermal transport in multilayer structures: A molecular dynamics study on Lennard-Jones solids. Frontiers of Physics, 2022, 17, .	2.4	8
448	Moving closer to experimental level materials property prediction using AI. Scientific Reports, 2022, 12, .	1.6	14
449	A simple descriptor for magnetic classification of 2D MXene materials. AIP Advances, 2022, 12, .	0.6	4
450	Improving Symbolic Regression for Predicting Materials Properties with Iterative Variable Selection. Journal of Chemical Theory and Computation, 2022, 18, 4945-4951.	2.3	11
451	Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery. ACS Catalysis, 2022, 12, 8572-8581.	5.5	18
452	The magnetic properties prediction and composition design of La-Co substitution Sr-hexaferrite based on high-through experiments and machine learning. Materials Today Communications, 2022, 32, 103996.	0.9	0
453	Machine learning assisted wrinkling design of hierarchical thin sheets. Computational Materials Science, 2022, 213, 111638.	1.4	1
454	Causal Paths Allowing Simultaneous Control of Multiple Nanoparticle Properties Using Multi-Target Bayesian Inference. Advanced Theory and Simulations, 2022, 5, .	1.3	2
455	Quantum embedding theories to simulate condensed systems on quantum computers. Nature Computational Science, 2022, 2, 424-432.	3.8	19



#	ARTICLE	IF	CITATIONS
474	Feature Fusion Deep Learning Model for Defects Prediction in Crystal Structures. <i>Crystals</i> , 2022, 12, 1324.	1.0	2
475	Treating Superhard Materials as Anomalies. <i>Journal of the American Chemical Society</i> , 2022, 144, 18075-18080.	6.6	8
476	Microstructure-Sensitive Uncertainty Quantification for Crystal Plasticity Finite Element Constitutive Models Using Stochastic Collocation Methods. <i>Frontiers in Materials</i> , 0, 9, .	1.2	7
477	Design of New Ternary Nitrides for Photovoltaic Applications via High-Throughput Calculations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 17398-17405.	1.5	1
478	Machine learning for battery research. <i>Journal of Power Sources</i> , 2022, 549, 232125.	4.0	22
479	The Rise of Catalysts Informatics. , 2022, , 349-371.		0
480	Automated performance analysis tools framework for HPC programs. <i>Procedia Computer Science</i> , 2022, 207, 1067-1076.	1.2	0
481	End-condition for solution small angle X-ray scattering measurements by kernel density estimation. <i>Science and Technology of Advanced Materials Methods</i> , 0, , .	0.4	0
482	A Knowledge Transfer Framework for General Alloy Materials Properties Prediction. <i>Materials</i> , 2022, 15, 7442.	1.3	1
483	Empowering engineering with data, machine learning and artificial intelligence: a short introductory review. <i>Advanced Modeling and Simulation in Engineering Sciences</i> , 2022, 9, .	0.7	9
484	High-throughput characterization methods for Ni-based superalloys and phase prediction via deep learning. <i>Journal of Materials Research and Technology</i> , 2022, 21, 1984-1997.	2.6	3
485	i-SISSO: Mutual information-based improved sure independent screening and sparsifying operator algorithm. <i>Engineering Applications of Artificial Intelligence</i> , 2022, 116, 105442.	4.3	4
486	Accelerating the adoption of research data management strategies. <i>Matter</i> , 2022, 5, 3614-3642.	5.0	2
487	Interpretable Graph Transformer Network for Predicting Adsorption Isotherms of Metal-Organic Frameworks. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5446-5456.	2.5	11
488	Modeling, optimization and understanding of adsorption process for pollutant removal via machine learning: Recent progress and future perspectives. <i>Chemosphere</i> , 2023, 311, 137044.	4.2	27
489	Multi-scale modeling of crystal-fluid interactions: State-of-the-art, challenges and prospects. , 2024, , 760-792.		1
490	Design of new Al-Si-Mg alloys by multi-modal mixed input simulation experiment. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2023, 72, 028101.	0.2	3
491	FAIR Big Data in the Materials Design Domain. , 2022, , 1-8.		4

#	ARTICLE	IF	CITATIONS
492	Data storage architectures to accelerate chemical discovery: data accessibility for individual laboratories and the community. <i>Chemical Science</i> , 2022, 13, 13646-13656.	3.7	9
493	Statistical mechanics in climate emulation: Challenges and perspectives. , 2022, 1, .		2
494	Superconductivity information extraction from the literature: A new corpus and its evaluations. <i>Advanced Engineering Informatics</i> , 2022, 54, 101768.	4.0	1
495	Generative Adversarial Networks and Mixture Density Networks-Based Inverse Modeling for Microstructural Materials Design. <i>Integrating Materials and Manufacturing Innovation</i> , 2022, 11, 637-647.	1.2	7
496	Machine learning (deep learning) and visualization assisted ferrite content prediction in austenitic stainless steel. <i>Materials Today Communications</i> , 2022, 33, 104943.	0.9	2
497	Toward autonomous laboratories: Convergence of artificial intelligence and experimental automation. <i>Progress in Materials Science</i> , 2023, 132, 101043.	16.0	19
498	State-of-the-Art Review on the Aspects of Martensitic Alloys Studied via Machine Learning. <i>Metals</i> , 2022, 12, 1884.	1.0	2
499	Electrochemoinformatics as an Emerging Scientific Field for Designing Materials and Electrochemical Energy Storage and Conversion Devices—An Application in Battery Science and Technology. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	4
500	Ultrafast inverse design of quantum dot optical spectra via a joint TD-DFT learning scheme and deep reinforcement learning. <i>AIP Advances</i> , 2022, 12, .	0.6	3
501	Machine learning for semiconductors. , 2022, 1, 100033.		6
502	Tellurium Treatment for the Modification of Sulfide Inclusions and Corresponding Industrial Applications in Special Steels: A Review. <i>Steel Research International</i> , 2023, 94, .	1.0	5
503	Phase Stability Through Machine Learning. <i>Journal of Phase Equilibria and Diffusion</i> , 2022, 43, 606-628.	0.5	2
504	Feature extended energy landscape model for interpreting coercivity mechanism. <i>Communications Physics</i> , 2022, 5, .	2.0	5
505	Machine learning accelerates the materials discovery. <i>Materials Today Communications</i> , 2022, 33, 104900.	0.9	11
506	Machine learning and materials informatics approaches for predicting transverse mechanical properties of unidirectional CFRP composites with microvoids. <i>Materials and Design</i> , 2022, 224, 111340.	3.3	29
507	Review on Perovskite-Type Compound Using Machine Learning. <i>Science of Advanced Materials</i> , 2022, 14, 1001-1017.	0.1	2
508	Using Machine Learning to make nanomaterials sustainable. <i>Science of the Total Environment</i> , 2023, 859, 160303.	3.9	10
509	Application of Machine Learning in Determining the Mechanical Properties of Materials. <i>Composites Science and Technology</i> , 2022, , 99-113.	0.4	12

#	ARTICLE	IF	CITATIONS
510	Neural network potentials for chemistry: concepts, applications and prospects. , 2023, 2, 28-58.		17
511	Machine-learning reveals the virtual screening strategies of solid hydrogen-bonded oligomeric assemblies for thermo-responsive applications. Chemical Engineering Journal, 2023, 456, 141073.	6.6	4
512	From jammed solids to mechanical metamaterials : A brief review. Current Opinion in Solid State and Materials Science, 2023, 27, 101053.	5.6	7
513	HADB: A materials-property database for hard-coating alloys. Thin Solid Films, 2023, 766, 139627.	0.8	1
514	Linking properties to microstructure in liquid metal embedded elastomers via machine learning. Computational Materials Science, 2023, 218, 111983.	1.4	1
515	Digital fingerprinting of microstructures. Computational Materials Science, 2023, 218, 111985.	1.4	2
516	Human-machine collaborative additive manufacturing. Journal of Manufacturing Systems, 2023, 66, 82-91.	7.6	10
517	Developing electron dynamics into a tool for 21st century chemistry simulations. Chemical Modelling, 2022, , 91-152.	0.2	1
518	Boosting-based model for solving Sm-Co alloy's maximum energy product prediction task. Archives of Materials Science and Engineering, 2022, 116, 71-80.	0.7	0
519	Predictive Analytics Approach for Steel Billets Quality Control System. , 2022, , .		0
520	Introducing materials informatics to dielectrics design. , 2022, , .		0
521	A systematic review of machine learning methods applied to fuel cells in performance evaluation, durability prediction, and application monitoring. International Journal of Hydrogen Energy, 2023, 48, 5197-5228.	3.8	42
522	Bayesian optimization of discrete dislocation plasticity of two-dimensional precipitation-hardened crystals. Physical Review Materials, 2022, 6, .	0.9	0
523	Bamboo phase quantification using thermogravimetric analysis: deconvolution and machine learning. Cellulose, 2023, 30, 1873-1893.	2.4	3
525	Intelligent Computing: The Latest Advances, Challenges, and Future. , 2023, 2, .		26
526	Predicting lattice thermal conductivity via machine learning: a mini review. Npj Computational Materials, 2023, 9, .	3.5	23
527	Predicting the Loading Parameters of a Square Panel Upon Linear Deflection. Proceedings in Adaptation, Learning and Optimization, 2023, , 84-91.	1.5	0
528	Transfer Learning in Inorganic Compounds's Crystal Structure Classification. Crystals, 2023, 13, 87.	1.0	0

#	ARTICLE	IF	CITATIONS
529	Metal AM process-structure-property relational linkages using Gaussian process surrogates. Additive Manufacturing, 2023, 62, 103398.	1.7	1
530	Bioresource Upgrade for Sustainable Energy, Environment, and Biomedicine. Nano-Micro Letters, 2023, 15, .	14.4	19
531	A secured big-data sharing platform for materials genome engineering: State-of-the-art, challenges and architecture. Future Generation Computer Systems, 2023, 142, 59-74.	4.9	4
532	Process Insights into Perovskite Thin-Film Photovoltaics from Machine Learning with In-Situ Luminescence Data. Solar Rrl, 2023, 7, .	3.1	4
533	Microstructure-Sensitive Material Design with Physics-Informed Neural Networks. , 2023, , .		0
534	Integrated data-driven modeling and experimental optimization of granular hydrogel matrices. Matter, 2023, 6, 1015-1036.	5.0	9
535	Rapid alloying in additive manufacturing using integrated computational materials engineering. , 2023, , 583-624.		1
536	Interpretable Machine Learning for Prediction of Post-Fire Self-Healing of Concrete. Materials, 2023, 16, 1273.	1.3	7
537	Water-soluble organic former selection for methane hydrates by supervised machine learning. Energy Reports, 2023, 9, 2935-2946.	2.5	3
539	GFlowNets for AI-driven scientific discovery. , 2023, 2, 557-577.		2
540	How to lead R&D digital transformation in a chemical corporation. MRS Advances, 2023, 8, 416-421.	0.5	1
541	An optimization of harmonic structure nickel-saving cryogenic steel via combinatorial high-throughput experiment. Journal of Iron and Steel Research International, 2023, 30, 1042-1049.	1.4	1
542	ET-AL: Entropy-targeted active learning for bias mitigation in materials data. Applied Physics Reviews, 2023, 10, .	5.5	5
543	Machine learning and visualization assisted solid solution strengthening phase prediction of high entropy alloys. Materials Today Communications, 2023, 35, 105894.	0.9	1
544	Stoichiometric growth of SrTiO3 films via Bayesian optimization with adaptive prior mean. , 2023, 1, .		1
545	Viruses as biomaterials. Materials Science and Engineering Reports, 2023, 153, 100715.	14.8	4
546	Bandgap energy prediction of senary zinblende III-V semiconductor compounds using machine learning. Materials Science in Semiconductor Processing, 2023, 161, 107461.	1.9	0
547	Data-Driven Design of Polymer-Based Biomaterials: High-throughput Simulation, Experimentation, and Machine Learning. ACS Applied Bio Materials, 2024, 7, 510-527.	2.3	11



#	ARTICLE	IF	CITATIONS
548	Prediction of the shear capacity of ultrahigh-performance concrete beams using neural network and genetic algorithm. <i>Scientific Reports</i> , 2023, 13, .	1.6	4
549	A two-step data augmentation method based on generative adversarial network for hardness prediction of high entropy alloy. <i>Computational Materials Science</i> , 2023, 220, 112064.	1.4	8
550	Modelling the dynamic physical properties of vulcanised polymer models by molecular dynamics simulations and machine learning. <i>Computational Materials Science</i> , 2023, 221, 112081.	1.4	1
551	Artificial Intelligence Approaches for Energetic Materials by Design: State of the Art, Challenges, and Future Directions. <i>Propellants, Explosives, Pyrotechnics</i> , 2023, 48, .	1.0	3
552	Multi-objective optimization of the epoxy matrix system using machine learning. <i>Results in Materials</i> , 2023, 17, 100376.	0.9	0
553	A deep learning convolutional neural network and multi-layer perceptron hybrid fusion model for predicting the mechanical properties of carbon fiber. <i>Materials and Design</i> , 2023, 227, 111760.	3.3	8
554	<i>CrystalMELA</i> : a new crystallographic machine learning platform for crystal system determination. <i>Journal of Applied Crystallography</i> , 2023, 56, 409-419.	1.9	2
556	Zero to zero nanoarchitectonics with fullerene: from molecules to nanoparticles. <i>Journal of Nanoparticle Research</i> , 2023, 25, .	0.8	2
557	Development of a machine learning model for prediction of continuous cooling transformation diagrams in welding heat-affected zone. <i>Journal of Materials Science</i> , 2023, 58, 4795-4808.	1.7	0
558	Symbolic Regression in Materials Science: Discovering Interatomic Potentials from Data. <i>Genetic and Evolutionary Computation</i> , 2023, , 1-30.	1.0	1
560	Summary of Efforts in Phase Prediction of High Entropy Alloys Using Machine Learning. , 2023, , 43-57.		0
561	MPpredictor: An Artificial Intelligence-Driven Web Tool for Composition-Based Material Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1865-1871.	2.5	8
562	An asynchronous parallel high-throughput model calibration framework for crystal plasticity finite element constitutive models. <i>Computational Mechanics</i> , 2023, 72, 485-498.	2.2	1
563	Artificial Intelligence in Physical Sciences: Symbolic Regression Trends and Perspectives. <i>Archives of Computational Methods in Engineering</i> , 2023, 30, 3845-3865.	6.0	13
564	Improving Scientific Image Processing Accessibility through Development of Graphic User Interfaces for scikit-image. , 0, , .		0
565	Neural Network as a Tool for Design of Amorphous Metal Alloys with Desired Elastoplastic Properties. <i>Metals</i> , 2023, 13, 812.	1.0	2
581	Machine learning methods in photochemistry and photophysics. , 2023, , 163-189.		2
602	Materials Science Ontology Design with Analytico-Synthetic Facet Analysis Framework. <i>Communications in Computer and Information Science</i> , 2023, , 211-221.	0.4	0



#	ARTICLE	IF	CITATIONS
610	Structural design of organic battery electrode materials: from DFT to artificial intelligence. Rare Metals, 2023, 42, 3269-3303.	3.6	1
622	AI for Learning Deformation Behavior of a Material: Predicting Stress-Strain Curves 4000x Faster Than Simulations. , 2023, , .		2
623	Pre-Activation based Representation Learning to Enhance Predictive Analytics on Small Materials Data. , 2023, , .		3
625	Which Deep Learning Framework Should I Use: A Comparative Study For Deep Regression Modeling. , 2022, , .		0
630	Physics-based Data-Augmented Deep Learning for Enhanced Autogenous Shrinkage Prediction on Experimental Dataset. , 2023, , .		2
631	An Introduction to Machine Learning in Molecular Sciences. Challenges and Advances in Computational Chemistry and Physics, 2023, , 1-19.	0.6	0
633	Machine Learning in Computer Aided Engineering. Computational Methods in Engineering & the Sciences, 2023, , 1-83.	0.3	0
638	Neural Networks for Constitutive Modeling: From Universal Function Approximators to Advanced Models and the Integration of Physics. Archives of Computational Methods in Engineering, 2024, 31, 1097-1127.	6.0	2
648	Advances of machine learning in materials science: Ideas and techniques. Frontiers of Physics, 2024, 19, .	2.4	0
650	Machine learning for analysis of experimental scattering and spectroscopy data in materials chemistry. Chemical Science, 2023, 14, 14003-14019.	3.7	3
658	A Study ofÂComparison Between YOLOv5 andÂYOLOv7 forÂDetection ofÂCracks inÂConcrete Structures. Lecture Notes in Electrical Engineering, 2024, , 489-500.	0.3	0
669	UNet Performance with Wafer Scale Engine (Optimization Case Study). , 2023, , .		0
699	Prediction of Mechanical Properties of Austenitic Stainless Steels with the Use of Synthetic Data via Generative Adversarial Networks. , 0, , .		0