Accelerated discovery of stable lead-free hybrid organic learning

Nature Communications

9, 3405

DOI: 10.1038/s41467-018-05761-w

Citation Report

#	Article	IF	Citations
1	Deep Learning for Nonadiabatic Excited-State Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 6702-6708.	2.1	126
2	Rationalizing Perovskite Data for Machine Learning and Materials Design. Journal of Physical Chemistry Letters, 2018, 9, 6948-6954.	2.1	68
3	Recent advances and applications of machine learning in solid-state materials science. Npj Computational Materials, 2019, 5, .	3.5	1,289
4	Rationalizing the interphase stability of Li|doped-Li₇La₃Zr₂O₁₂via automated reaction screening and machine learning. Journal of Materials Chemistry A, 2019, 7, 19961-19969.	5.2	59
5	Solar steam generation based on the photothermal effect: from designs to applications, and beyond. Journal of Materials Chemistry A, 2019, 7, 19203-19227.	5.2	175
6	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 2019, 10, 7913-7922.	3.7	129
7	Predicting the onset temperature (Tg) of Ge Se1â^' glass transition: a feature selection based two-stage support vector regression method. Science Bulletin, 2019, 64, 1195-1203.	4.3	41
8	Learn-and-Match Molecular Cations for Perovskites. Journal of Physical Chemistry A, 2019, 123, 7323-7334.	1.1	28
9	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. Journal of Materials Chemistry A, 2019, 7, 17480-17488.	5.2	80
10	Accelerated Discovery of Two-Dimensional Optoelectronic Octahedral Oxyhalides via High-Throughput Ab Initio Calculations and Machine Learning. Journal of Physical Chemistry Letters, 2019, 10, 6734-6740.	2.1	40
11	Predictions and Strategies Learned from Machine Learning to Develop Highâ€Performing Perovskite Solar Cells. Advanced Energy Materials, 2019, 9, 1901891.	10.2	83
12	Accelerated Design of Catalytic Water-Cleaning Nanomotors via Machine Learning. ACS Applied Materials & Interfaces, 2019, 11, 40099-40106.	4.0	33
13	Accelerated Search for BaTiO₃â€Based Ceramics with Large Energy Storage at Low Fields Using Machine Learning and Experimental Design. Advanced Science, 2019, 6, 1901395.	5.6	44
14	Machine learning in materials science. InformaÄnÃ-MateriÃ¡ly, 2019, 1, 338-358.	8.5	427
15	Machine learningâ€“assisted molecular design and efficiency prediction for high-performance organic photovoltaic materials. Science Advances, 2019, 5, eaay4275.	4.7	181
16	Unraveling Correlations between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning. Journal of Physical Chemistry Letters, 2019, 10, 7277-7284.	2.1	65
17	Virtual Issue on Machine-Learning Discoveries in Materials Science. Chemistry of Materials, 2019, 31, 8243-8247.	3.2	23
18	The inverse design of structural color using machine learning. Nanoscale, 2019, 11, 21748-21758.	2.8	50

#	Article	IF	Citations
19	Physical metallurgy-guided machine learning and artificial intelligent design of ultrahigh-strength stainless steel. Acta Materialia, 2019, 179, 201-214.	3.8	140
20	Global discovery of stable and non-toxic hybrid organic-inorganic perovskites for photovoltaic systems by combining machine learning method with first principle calculations. Nano Energy, 2019, 66, 104070.	8.2	48
21	Emerging role of machine learning in light-matter interaction. Light: Science and Applications, 2019, 8, 84.	7.7	56
22	Materials informatics: From the atomic-level to the continuum. Acta Materialia, 2019, 168, 473-510.	3.8	108
23	Rapid Discovery of Ferroelectric Photovoltaic Perovskites and Material Descriptors via Machine Learning. Small Methods, 2019, 3, 1900360.	4.6	76
24	Perovskites with d-block metals for solar energy applications. Dalton Transactions, 2019, 48, 9516-9537.	1.6	24
25	Centimeter-size square 2D layered Pb-free hybrid perovskite single crystal (CH₃NH₃)₂MnCl₄ for red photoluminescence. CrystEngComm, 2019, 21, 4085-4091.	1.3	31
26	High-throughput computational design of organicâ€“inorganic hybrid halide semiconductors beyond perovskites for optoelectronics. Energy and Environmental Science, 2019, 12, 2233-2243.	15.6	82
27	MA₂CoBr₄: lead-free cobalt-based perovskite for electrochemical conversion of water to oxygen. Chemical Communications, 2019, 55, 6779-6782.	2.2	13
28	Halide Perovskite Nanocrystals for Nextâ€Generation Optoelectronics. Small, 2019, 15, e1900801.	5.2	48
29	Hybrid organic-inorganic perovskites: Polar properties and applications. Coordination Chemistry Reviews, 2019, 387, 398-414.	9.5	84
30	Theoretical Prediction of Chiral 3D Hybrid Organicâ€“Inorganic Perovskites. Advanced Materials, 2019, 31, e1807628.	11.1	64
31	Water in hybrid perovskites: Bulk MAPbI3 degradation via super-hydrous state. APL Materials, 2019, 7, .	2.2	42
32	Emerging Theory, Materials, and Screening Methods: New Opportunities for Promoting Thermoelectric Performance. Annalen Der Physik, 2019, 531, 1800437.	0.9	83
33	From DFT to machine learning: recent approaches to materials scienceâ€“a review. JPhys Materials, 2019, 2, 032001.	1.8	385
34	Unsupervised discovery of solid-state lithium ion conductors. Nature Communications, 2019, 10, 5260.	5.8	150
35	Activity Origin and Design Principles for Oxygen Reduction on Dual-Metal-Site Catalysts: A Combined Density Functional Theory and Machine Learning Study. Journal of Physical Chemistry Letters, 2019, 10, 7760-7766.	2.1	149
36	Machine Learning Constrained with Dimensional Analysis and Scaling Laws: Simple, Transferable, and Interpretable Models of Materials from Small Datasets. Chemistry of Materials, 2019, 31, 314-321.	3.2	23

#	Article	IF	Citations
37	Guiding Principles for Designing Highly Efficient Metalâ€Free Carbon Catalysts. Advanced Materials, 2019, 31, e1805252.	11.1	110
38	Simulation and design of energy materials accelerated by machine learning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1421.	6.2	41
39	Tin Halide Perovskites: Progress and Challenges. Advanced Energy Materials, 2020, 10, 1902584.	10.2	124
40	Autonomous Discovery in the Chemical Sciences Partâ€…I: Progress. Angewandte Chemie - International Edition, 2020, 59, 22858-22893.	7.2	180
41	Robust random forest based non-fullerene organic solar cells efficiency prediction. Organic Electronics, 2020, 76, 105465.	1.4	48
42	A high throughput molecular screening for organic electronics via machine learning: present status and perspective. Japanese Journal of Applied Physics, 2020, 59, SD0801.	0.8	43
43	Autonome Entdeckung in den chemischen Wissenschaften, Teilâ€…I: Fortschritt. Angewandte Chemie, 2020, 132, 23054-23091.	1.6	11
44	Enumeration of de novo inorganic complexes for chemical discovery and machine learning. Molecular Systems Design and Engineering, 2020, 5, 139-152.	1.7	23
45	Application of fuzzy learning in the research of binary alloys: Revisit and validation. Computational Materials Science, 2020, 172, 109350.	1.4	5
46	Recent advances in two-dimensional ferromagnetism: materials synthesis, physical properties and device applications. Nanoscale, 2020, 12, 2309-2327.	2.8	67
47	Machine-learning-assisted screening of pure-silica zeolites for effective removal of linear siloxanes and derivatives. Journal of Materials Chemistry A, 2020, 8, 3228-3237.	5.2	14
48	A steel property optimization model based on the XGBoost algorithm and improved PSO. Computational Materials Science, 2020, 174, 109472.	1.4	117
49	Machine learning analysis on stability of perovskite solar cells. Solar Energy Materials and Solar Cells, 2020, 205, 110284.	3.0	53
50	Exploiting Ionic Radii for Rational Design of Halide Perovskites. Chemistry of Materials, 2020, 32, 595-604.	3.2	50
51	Tensile property prediction by feature engineering guided machine learning in reduced activation ferritic/martensitic steels. Journal of Nuclear Materials, 2020, 529, 151823.	1.3	27
52	Predicting Inorganic Photovoltaic Materials with Efficiencies >26% via Structure-Relevant Machine Learning and Density Functional Calculations. Cell Reports Physical Science, 2020, 1, 100179.	2.8	20
53	Machine learning for halide perovskite materials. Nano Energy, 2020, 78, 105380.	8.2	65
54	Material platforms for defect qubits and single-photon emitters. Applied Physics Reviews, 2020, 7, .	5.5	96

#	Article	IF	Citations
55	Engineering early prediction of supercapacitorsâ€™ cycle life using neural networks. Materials Today Energy, 2020, 18, 100537.	2.5	14
56	Element Code from Pseudopotential as Efficient Descriptors for a Machine Learning Model to Explore Potential Lead-Free Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 8914-8921.	2.1	11
57	Extracting bulk defect parameters in silicon wafers using machine learning models. Npj Computational Materials, 2020, 6, .	3.5	10
58	Simple descriptor derived from symbolic regression accelerating the discovery of new perovskite catalysts. Nature Communications, 2020, 11, 3513.	5.8	184
59	Machine learning-driven new material discovery. Nanoscale Advances, 2020, 2, 3115-3130.	2.2	111
60	AI Applications through the Whole Life Cycle of Material Discovery. Matter, 2020, 3, 393-432.	5.0	86
61	A machine learning scheme for the catalytic activity of alloys with intrinsic descriptors. Journal of Materials Chemistry A, 2020, 8, 17507-17515.	5.2	60
62	Method construction of structure-property relationships from data by machine learning assisted mining for materials design applications. Materials and Design, 2020, 196, 109194.	3.3	24
63	Evaluation-oriented exploration of photo energy conversion systems: from fundamental optoelectronics and material screening to the combination with data science. Polymer Journal, 2020, 52, 1307-1321.	1.3	43
64	A Machine Learning Model on Simple Features for CO₂ Reduction Electrocatalysts. Journal of Physical Chemistry C, 2020, 124, 22471-22478.	1.5	125
65	Knowledge-Based Descriptor for the Compositional Dependence of the Phase Transition in BaTiO₃-Based Ferroelectrics. ACS Applied Materials & Interfaces, 2020, 12, 44970-44980.	4.0	7
66	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	5.8	57
67	Deep Mining Stable and Nontoxic Hybrid Organicâ€“Inorganic Perovskites for Photovoltaics via Progressive Machine Learning. ACS Applied Materials & Interfaces, 2020, 12, 57821-57831.	4.0	20
68	Computational high throughput screening of inorganic cation based halide perovskites for perovskite only tandem solar cells. Materials Research Express, 2020, 7, 055502.	0.8	19
69	Coupling a Crystal Graph Multilayer Descriptor to Active Learning for Rapid Discovery of 2D Ferromagnetic Semiconductors/Halfâ€Metals/Metals. Advanced Materials, 2020, 32, e2002658.	11.1	86
70	Optimization of thermal conductivity of UO2â€“Mo composite with continuous Mo channel based on finite element method and machine learning. International Journal of Heat and Mass Transfer, 2020, 159, 120067.	2.5	15
71	Opportunities and Challenges for Machine Learning in Materials Science. Annual Review of Materials Research, 2020, 50, 71-103.	4.3	183
72	Robot-Accelerated Perovskite Investigation and Discovery. Chemistry of Materials, 2020, 32, 5650-5663.	3.2	113

#	Article	IF	Citations
73	Bayesian optimization based on a unified figure of merit for accelerated materials screening: A case study of halide perovskites. Science China Materials, 2020, 63, 1024-1035.	3.5	25
74	Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization. ACS Central Science, 2020, 6, 513-524.	5.3	114
75	Chiral-perovskite optoelectronics. Nature Reviews Materials, 2020, 5, 423-439.	23.3	445
76	Hot Carriers in Halide Perovskites: How Hot Truly?. Journal of Physical Chemistry Letters, 2020, 11, 2743-2750.	2.1	41
77	Designing bioinspired brick-and-mortar composites using machine learning and statistical learning. Communications Materials, 2020, 1, .	2.9	17
78	An Adaptive Machine Learning Strategy for Accelerating Discovery of Perovskite Electrocatalysts. ACS Catalysis, 2020, 10, 4377-4384.	5.5	75
79	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. Journal of Physical Chemistry A, 2020, 124, 3286-3299.	1.1	48
80	Machine Learning for Predicting the Band Gaps of ABX₃ Perovskites from Elemental Properties. Journal of Physical Chemistry C, 2020, 124, 8905-8918.	1.5	99
81	Importance of structural deformation features in the prediction of hybrid perovskite bandgaps. Computational Materials Science, 2020, 184, 109858.	1.4	22
82	Metal-Free Hybrid Organicâ€“Inorganic Perovskites for Photovoltaics. Journal of Physical Chemistry Letters, 2020, 11, 5938-5947.	2.1	12
83	Perspective on theoretical methods and modeling relating to electro-catalysis processes. Chemical Communications, 2020, 56, 9937-9949.	2.2	52
84	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. Advanced Theory and Simulations, 2020, 3, 2000022.	1.3	10
85	Machine Learning Based Distinguishing between Ferroelectric and Nonâ€Ferroelectric Polarizationâ€“Electric Field Hysteresis Loops. Advanced Theory and Simulations, 2020, 3, 2000106.	1.3	3
86	Magnetic twoâ€dimensional layered crystals meet with ferromagnetic semiconductors. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 639-655.	8.5	76
87	Using machine learning and feature engineering to characterize limited material datasets of high-entropy alloys. Computational Materials Science, 2020, 175, 109618.	1.4	102
88	Stability diagrams, defect tolerance, and absorption coefficients of hybrid halide semiconductors: High-throughput first-principles characterization. Journal of Chemical Physics, 2020, 152, 084106.	1.2	22
89	Artificial Intelligence to Power the Future of Materials Science and Engineering. Advanced Intelligent Systems, 2020, 2, 1900143.	3.3	75
90	Machine learning: Accelerating materials development for energy storage and conversion. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 553-576.	8.5	212

#	Article	IF	Citations
91	Feature Engineering of Solidâ€State Crystalline Lattices for Machine Learning. Advanced Theory and Simulations, 2020, 3, 1900190.	1.3	3
92	Multiâ€Layer Feature Selection Incorporating Weighted Scoreâ€Based Expert Knowledge toward Modeling Materials with Targeted Properties. Advanced Theory and Simulations, 2020, 3, 1900215.	1.3	74
93	Computational functionalityâ€driven design of semiconductors for optoelectronic applications. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 879-904.	8.5	32
94	Temperature-Dependent Dynamic Carrier Process of FAPbI₃ Nanocrystalsâ€™ Film. Journal of Physical Chemistry C, 2020, 124, 5093-5098.	1.5	14
95	Bi-directional prediction of structural characteristics and effective thermal conductivities of composite fuels through learning from finite element simulation results. Materials and Design, 2020, 189, 108483.	3.3	14
96	A progressive learning method for predicting the band gap of ABO₃ perovskites using an instrumental variable. Journal of Materials Chemistry C, 2020, 8, 3127-3136.	2.7	23
97	A Critical Review of Machine Learning of Energy Materials. Advanced Energy Materials, 2020, 10, 1903242.	10.2	319
98	Lowâ€dimensional metal halide perovskites and related optoelectronic applications. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 341-378.	8.5	72
99	Machine learning of octahedral tilting in oxide perovskites by symbolic classification with compressed sensing. Computational Materials Science, 2020, 180, 109690.	1.4	19
100	Zeolite Adsorption Isotherms Predicted by Pore Channel and Local Environmental Descriptors: Feature Learning on DFT Binding Strength. Journal of Physical Chemistry C, 2020, 124, 9314-9328.	1.5	12
101	Property-Oriented Material Design Based on a Data-Driven Machine Learning Technique. Journal of Physical Chemistry Letters, 2020, 11, 3920-3927.	2.1	54
102	Discovery of Novel Two-Dimensional Photovoltaic Materials Accelerated by Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 3075-3081.	2.1	35
103	Accelerated Discovery of Potential Organic Dyes for Dyeâ€Sensitized Solar Cells by Interpretable Machine Learning Models and Virtual Screening. Solar Rrl, 2020, 4, 2000110.	3.1	35
104	Highâ€throughput computational materials screening and discovery of optoelectronic semiconductors. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	6.2	52
105	Two-dimensional Janus material MoS2(1-x)Se2x (0Â<ÂxÂ<Â1) for photovoltaic applications: A machine learning and density functional study. Computational Materials Science, 2021, 186, 109998.	1.4	9
106	Potential replacement to lead: Alkali metal potassium and transition metal zinc in organo-metal halide perovskite materials. Journal of Alloys and Compounds, 2021, 861, 158207.	2.8	3
107	Accelerated discovery of stable spinels in energy systems via machine learning. Nano Energy, 2021, 81, 105665.	8.2	30
108	2D Hybrid Halide Perovskites: Synthesis, Properties, and Applications. Solar Rrl, 2021, 5, .	3.1	20

#	Article	IF	Citations
109	Engineered two-dimensional nanomaterials: an emerging paradigm for water purification and monitoring. Materials Horizons, 2021, 8, 758-802.	6.4	92
110	Lowâ€Dimensional Metal Halide Perovskite Photodetectors. Advanced Materials, 2021, 33, e2003309.	11.1	319
111	Determining Multiâ€Component Phase Diagrams with Desired Characteristics Using Active Learning. Advanced Science, 2021, 8, 2003165.	5.6	23
112	Critical review of machine learning applications in perovskite solar research. Nano Energy, 2021, 80, 105546.	8.2	70
113	Highâ€throughput computational design of halide perovskites and beyond for optoelectronics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1500.	6.2	16
114	Metal halide perovskites for light-emitting diodes. Nature Materials, 2021, 20, 10-21.	13.3	800
115	A new material discovery platform of stable layered oxide cathodes for K-ion batteries. Energy and Environmental Science, 2021, 14, 5864-5874.	15.6	30
116	Accelerated design of promising mixed lead-free double halide organicâ€“inorganic perovskites for photovoltaics using machine learning. Nanoscale, 2021, 13, 12250-12259.	2.8	21
117	matExplorer: Visual Exploration on Predicting Ionic Conductivity for Solid-state Electrolytes. IEEE Transactions on Visualization and Computer Graphics, 2022, 28, 65-75.	2.9	5
118	Prediction of band gap for 2D hybrid organicâ€“inorganic perovskites by using machine learning through molecular graphics descriptors. New Journal of Chemistry, 2021, 45, 9427-9433.	1.4	11
119	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. Physical Review B, 2021, 103, .	1.1	16
120	Low-energy ferroelectricâ€“paraelectric phase transitions of three-dimensional A(II)B(I)X3-type perovskite ferroelectrics: How to realize high phase transition temperatures. APL Materials, 2021, 9, .	2.2	5
121	Metalâ€Free Organic Halide Perovskite: A New Class for Next Optoelectronic Generation Devices. Advanced Energy Materials, 2021, 11, 2003331.	10.2	29
122	Predicting the Electronic and Structural Properties of Two-Dimensional Materials Using Machine Learning. Computers, Materials and Continua, 2021, 67, 1287-1300.	1.5	3
123	Hierarchical computational screening of layered lead-free metal halide perovskites for optoelectronic applications. Journal of Materials Chemistry A, 2021, 9, 6476-6486.	5.2	15
124	A universal screening strategy for the accelerated design of superior oxygen evolution/reduction electrocatalysts. Journal of Materials Chemistry A, 2021, 9, 3511-3519.	5.2	21
125	Data-driven machine learning model for the prediction of oxygen vacancy formation energy of metal oxide materials. Physical Chemistry Chemical Physics, 2021, 23, 15675-15684.	1.3	8
126	Experimentâ€Oriented Machine Learning of Polymer:Nonâ€Fullerene Organic Solar Cells. Advanced Functional Materials, 2021, 31, 2011168.	7.8	42

#	Article	IF	Citations
127	Photovoltaic neurointerface based on aluminum antimonide nanocrystals. Communications Materials, 2021, 2, .	2.9	23
128	Topological representations of crystalline compounds for the machine-learning prediction of materials properties. Npj Computational Materials, 2021, 7, .	3.5	36
129	2D Materials Bridging Experiments and Computations for Electro/Photocatalysis. Advanced Energy Materials, 2022, 12, 2003841.	10.2	116
130	Recent progress of mesoporous materials for high performance supercapacitors. Microporous and Mesoporous Materials, 2021, 314, 110870.	2.2	40
131	Efficient sampling for decision making in materials discovery*. Chinese Physics B, 2021, 30, 050705.	0.7	4
132	Machine learning for advanced energy materials. Energy and AI, 2021, 3, 100049.	5.8	96
133	High-performance quasi-2D perovskite light-emitting diodes: from materials to devices. Light: Science and Applications, 2021, 10, 61.	7.7	235
134	Molecular Design of Three-Dimensional Metal-Free A(NH₄)X₃ Perovskites for Photovoltaic Applications. Jacs Au, 2021, 1, 475-483.	3.6	19
135	Current Methods of Power Conversion Efficiency Optimization for Perovskite Solar Cells. , 2021, , .		0
136	Perspectiveâ€"Accelerated Discovery of Organic-Inorganic Hybrid Materials via Machine Learning. ECS Journal of Solid State Science and Technology, 2021, 10, 037001.	0.9	1
137	Applying machine learning to balance performance and stability of high energy density materials. IScience, 2021, 24, 102240.	1.9	28
138	Machine Learning Model for High-Throughput Screening of Perovskite Manganites with the Highest NÃ©el Temperature. Journal of Superconductivity and Novel Magnetism, 2021, 34, 1961-1969.	0.8	3
139	Microstructure Maps of Complex Perovskite Materials from Extensive Monte Carlo Sampling Using Machine Learning Enabled Energy Model. Journal of Physical Chemistry Letters, 2021, 12, 3591-3599.	2.1	16
140	Machine learning and descriptor selection for the computational discovery of metal-organic frameworks. Molecular Simulation, 0, , 1-21.	0.9	29
141	Prediction of Mechanical Properties of Wrought Aluminium Alloys Using Feature Engineering Assisted Machine Learning Approach. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2021, 52, 2873-2884.	1.1	22
142	Data-driven enhancement of cubic phase stability in mixed-cation perovskites. Machine Learning: Science and Technology, 2021, 2, 025030.	2.4	17
143	Machine Learning Boosts the Design and Discovery of Nanomaterials. ACS Sustainable Chemistry and Engineering, 2021, 9, 6130-6147.	3.2	44
145	Programmable Logic in Metalâ€"Organic Frameworks for Catalysis. Advanced Materials, 2021, 33, e2007442.	11.1	129

#	Article	IF	Citations
146	Deep exploration of random forest model boosts the interpretability of machine learning studies of complicated immune responses and lung burden of nanoparticles. Science Advances, 2021, 7, .	4.7	71
147	Recent advancements in halide perovskite nanomaterials and their optoelectronic applications. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 962-986.	8.5	25
148	Machine learning identified materials descriptors for ferroelectricity. Acta Materialia, 2021, 209, 116815.	3.8	33
149	NNIâ€šSMOTEâ€XGBoost: A Novel Small Sample Analysis Method for Properties Prediction of Polymer Materials. Macromolecular Theory and Simulations, 2021, 30, 2100010.	0.6	15
150	Molecular excited states through a machine learning lens. Nature Reviews Chemistry, 2021, 5, 388-405.	13.8	107
151	Predicting inorganic dimensionality in templated metal oxides. Journal of Chemical Physics, 2021, 154, 184708.	1.2	6
152	Alternative Loneâ€Pair ns²â€Cationâ€Based Semiconductors beyond Lead Halide Perovskites for Optoelectronic Applications. Advanced Materials, 2021, 33, e2008574.	11.1	34
153	Encoding the atomic structure for machine learning in materials science. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1558.	6.2	29
154	Comparative analysis of machine learning approaches on the prediction of the electronic properties of perovskites: A case study of ABX3 and A2BBâ€™X6. Materials Today Communications, 2021, 27, 102462.	0.9	11
155	Predicting the Formability of Hybrid Organicâ€“Inorganic Perovskites via an Interpretable Machine Learning Strategy. Journal of Physical Chemistry Letters, 2021, 12, 7423-7430.	2.1	36
156	Advances in Near-Infrared Luminescent Materials without Cr³⁺: Crystal Structure Design, Luminescence Properties, and Applications. Chemistry of Materials, 2021, 33, 5496-5526.	3.2	76
157	Catalyze Materials Science with Machine Learning. , 2021, 3, 1151-1171.		28
158	The Advantage of Nanowire Configuration in Band Structure Determination. Advanced Functional Materials, 2021, 31, 2105426.	7.8	4
159	Machine learning and symbolic regression investigation on stability of MXene materials. Computational Materials Science, 2021, 196, 110578.	1.4	26
160	Predictive Design Model for Low-Dimensional Organicâ€“Inorganic Halide Perovskites Assisted by Machine Learning. Journal of the American Chemical Society, 2021, 143, 12766-12776.	6.6	68
161	Machine-Learning Approach for Predicting the Discharging Capacities of Doped Lithium Nickelâ€“Cobaltâ€“Manganese Cathode Materials in Li-Ion Batteries. ACS Central Science, 2021, 7, 1551-1560.	5.3	27
162	High-performance chemical information database towards accelerating discovery of metal-organic frameworks for gas adsorption with machine learning. Chinese Journal of Chemical Physics, 2021, 34, 436-442.	0.6	1
163	Graph representational learning for bandgap prediction in varied perovskite crystals. Computational Materials Science, 2021, 196, 110530.	1.4	16

#	Article	IF	Citations
164	Unsupervised discovery of thin-film photovoltaic materials from unlabeled data. Npj Computational Materials, 2021, 7, .	3.5	13
165	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
166	Efficient Modeling Workflow for Accurate Electronic Structures of Hybrid Perovskites. Journal of Physical Chemistry C, 2021, 125, 18597-18603.	1.5	8
167	Synthesizable Double Perovskite Oxide Search via Machine Learning and Highâ€Throughput Computational Screening. Advanced Theory and Simulations, 2021, 4, 2100263.	1.3	14
168	Gold Segregation Improves Electrocatalytic Activity of Icosahedron Au@Pt Nanocluster: Insights from Machine Learning â€. Chinese Journal of Chemistry, 0, , .	2.6	10
169	A coupled machine learning and genetic algorithm approach to the design of porous electrodes for redox flow batteries. Applied Energy, 2021, 298, 117177.	5.1	35
170	A geometric-information-enhanced crystal graph network for predicting properties of materials. Communications Materials, 2021, 2, .	2.9	27
171	Machine learning prediction of stability, topological properties and band gap of topological insulators in tetradymites. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 409, 127508.	0.9	0
172	Use of metamodels for rapid discovery of narrow bandgap oxide photocatalysts. IScience, 2021, 24, 103068.	1.9	17
173	Applied Machine Learning for Developing Nextâ€Generation Functional Materials. Advanced Functional Materials, 2021, 31, 2104195.	7.8	28
174	Relationships between Distortions of Inorganic Framework and Band Gap of Layered Hybrid Halide Perovskites. Chemistry of Materials, 2021, 33, 7518-7526.	3.2	22
175	Artificial Intelligence Designer for Highly-Efficient Organic Photovoltaic Materials. Journal of Physical Chemistry Letters, 2021, 12, 8847-8854.	2.1	15
176	Compositionâ€Dependent Photoluminescence Properties and Antiâ€Counterfeiting Applications of A₂AgX₃ (AÂ=ÂRb, Cs; XÂ= ÂCl, Br, I). Advanced Functional Materials, 2021, 31, 2104941.	7.8	50
177	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. Npj Computational Materials, 2021, 7, .	3.5	19
178	Machine learning aided design of perovskite oxide materials for photocatalytic water splitting. Journal of Energy Chemistry, 2021, 60, 351-359.	7.1	68
179	Discovery of marageing steels: machine learning vs. physical metallurgical modelling. Journal of Materials Science and Technology, 2021, 87, 258-268.	5.6	8
180	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. Science Bulletin, 2021, 66, 1973-1985.	4.3	32
181	Machine-learning based design of digital materials for elastic wave control. Extreme Mechanics Letters, 2021, 48, 101372.	2.0	16

#	Article	IF	Citations
182	Phase segmentation of uncured prepreg X-Ray CT micrographs. Composites Part A: Applied Science and Manufacturing, 2021, 149, 106527.	3.8	10
183	Improved physics-based structural descriptors of perovskite materials enable higher accuracy of machine learning. Computational Materials Science, 2021, 198, 110714.	1.4	11
184	A Machine Learning Shortcut for Screening the Spinel Structures of Mg/Zn Ion Battery Cathodes with a High Conductivity and Rapid Ion Kinetics. Energy Storage Materials, 2021, 42, 277-285.	9.5	18
185	Key factors governing the device performance of CIGS solar cells: Insights from machine learning. Solar Energy, 2021, 228, 45-52.	2.9	14
186	Recent machine learning guided material research - A review. Computational Condensed Matter, 2021, 29, e00597.	0.9	4
187	Screening for lead-free inorganic double perovskites with suitable band gaps and high stability using combined machine learning and DFT calculation. Applied Surface Science, 2021, 568, 150916.	3.1	38
188	Is machine learning redefining the perovskite solar cells?. Journal of Energy Chemistry, 2022, 66, 74-90.	7.1	27
189	Voting Data-Driven Regression Learning for Accelerating Discovery of Advanced Functional Materials and Applications to Two-Dimensional Ferroelectric Materials. Journal of Physical Chemistry Letters, 2021, 12, 973-981.	2.1	11
190	Predicting adsorption ability of adsorbents at arbitrary sites for pollutants using deep transfer learning. Npj Computational Materials, 2021, 7, .	3.5	22
191	Machine Learning Accelerated Insights of Perovskite Materials. Springer Series in Materials Science, 2021, , 197-223.	0.4	0
192	Training a Model for PredictingAdsorption Energy of Metal Ions Based on Machine Learning. Wuji Cailiao Xuebao/Journal of Inorganic Materials, 2021, , 748.	0.6	2
193	Discovery of Lead-Free Hybrid Organic/Inorganic Perovskites Using Metaheuristic-Driven DFT Calculations. Chemistry of Materials, 2021, 33, 782-798.	3.2	23
194	Machine learning for perovskite materials design and discovery. Npj Computational Materials, 2021, 7, .	3.5	189
195	Data-driven analysis of the electronic-structure factors controlling the work functions of perovskite oxides. Physical Chemistry Chemical Physics, 2021, 23, 6880-6887.	1.3	7
197	Directly predicting limiting potentials from easily obtainable physical properties of graphene-supported single-atom electrocatalysts by machine learning. Journal of Materials Chemistry A, 2020, 8, 5663-5670.	5.2	112
198	Machine learning in materials design: Algorithm and application*. Chinese Physics B, 2020, 29, 116103.	0.7	24
199	Machine Learning for Predicting Perovskite Solar Cell Opto-Electronic Properties. , 2020, , .		4
200	Machine Learning in Materials Discovery: Confirmed Predictions and Their Underlying Approaches. Annual Review of Materials Research, 2020, 50, 49-69.	4.3	75

#	Article	IF	Citations
201	Synthesis of Sb(V) Complexes with Pyridyl Cations and Application for Lead-free Perovskite Solar Cells. Chemistry Letters, 2020, 49, 944-946.	0.7	1
202	Predictive and generative machine learning models for photonic crystals. Nanophotonics, 2020, 9, 4183-4192.	2.9	58
203	Tin Halide Perovskites: From Fundamental Properties to Solar Cells. Advanced Materials, 2022, 34, e2105844.	11.1	124
204	Knowledge-driven material design platform based on the whole-process simulation and modeling. International Journal of Modeling, Simulation, and Scientific Computing, 0, , .	0.9	1
205	Machine Learning Accelerates the Discovery of Light-Absorbing Materials for Double Perovskite Solar Cells. Journal of Physical Chemistry C, 2021, 125, 22483-22492.	1.5	16
206	Machine Learning Driven Synthesis of Few-Layered WTe₂ with Geometrical Control. Journal of the American Chemical Society, 2021, 143, 18103-18113.	6.6	30
207	Innovative Materials Science via Machine Learning. Advanced Functional Materials, 2022, 32, 2108044.	7.8	67
208	Graph network based deep learning of bandgaps. Journal of Chemical Physics, 2021, 155, 154702.	1.2	12
209	Novel Materials for Urban Farming. Advanced Materials, 2022, 34, e2105009.	11.1	24
210	Computer-aided synthesis of cost-effective perovskite crystals: an emerging alternative to silicon solar cells. Clean Technologies and Environmental Policy, 2020, 22, 1187-1198.	2.1	3
211	Artificial intelligence: A powerful paradigm for scientific research. Innovation(China), 2021, 2, 100179.	5.2	200
212	Accurate bandgap predictions of solids assisted by machine learning. Materials Today Communications, 2021, 29, 102932.	0.9	11
213	Machine learning phases and criticalities without using real data for training. Physical Review B, 2020, 102, .	1.1	8
214	Balancing data for generalizable machine learning to predict glass-forming ability of ternary alloys. Scripta Materialia, 2022, 209, 114366.	2.6	21
215	A universal neural network for learning phases. European Physical Journal Plus, 2021, 136, 1.	1.2	10
216	Molecular Bond Engineering and Feature Learning for the Design of Hybrid Organicâ€“Inorganic Perovskite Solar Cells with Strong Noncovalent Halogenâ€“Cation Interactions. Journal of Physical Chemistry C, 2021, 125, 25316-25326.	1.5	6
217	Predicting Perovskite Bandgap and Solar Cell Performance with Machine Learning. Solar Rrl, 2022, 6, 2100927.	3.1	12
218	Machine Learning Applications for The Tensile Property Evaluation of Steel: An Overview. , 2022, , 1-18.		0

#	Article	IF	Citations
219	On-the-fly interpretable machine learning for rapid discovery of two-dimensional ferromagnets with high Curie temperature. CheM, 2022, 8, 769-783.	5.8	38
220	Shedding light on the energy applications of emerging 2D hybrid organic-inorganic halide perovskites. IScience, 2022, 25, 103753.	1.9	9
221	Study on bandgap predications of ABX3-type perovskites by machine learning. Organic Electronics, 2022, 101, 106426.	1.4	21
223	A Genetic Algorithm-Based Artificial Network Method for Material Feature Recombination. , 2021, , .		0
224	Unveiling the layer-dependent electronic properties in transition-metal dichalcogenide heterostructures assisted by machine learning. Nanoscale, 2022, 14, 2511-2520.	2.8	6
225	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure. Physical Review Letters, 2022, 128, 047001.	2.9	91
226	Î”-Machine learning-driven discovery of double hybrid organicâ€“inorganic perovskites. Journal of Materials Chemistry A, 2022, 10, 1402-1413.	5.2	12
227	Disentangling the effect of doping chemistry on the energy storage property of barium titanate ferroelectrics via data science tools. Journal of Materials Chemistry C, 0, , .	2.7	1
228	A collaborative design platform for new alloy material development. Advanced Engineering Informatics, 2022, 51, 101488.	4.0	8
229	Highly accurate machine learning prediction of crystal point groups for ternary materials from chemical formula. Scientific Reports, 2022, 12, 1577.	1.6	9
230	DiSCoVeR: a materials discovery screening tool for high performance, unique chemical compositions. , 2022, 1, 226-240.		11
231	Predicting the photon energy of quasi-2D lead halide perovskites from the precursor composition through machine learning. Nanoscale Advances, 2022, 4, 1632-1638.	2.2	6
232	Data-driven design of novel halide perovskite alloys. Energy and Environmental Science, 2022, 15, 1930-1949.	15.6	26
233	Classification of magnetic ground states and prediction of magnetic moments of inorganic magnetic materials based on machine learning. Wuli Xuebao/Acta Physica Sinica, 2022, 71, 060202.	0.2	4
234	Industrial IoT-Enabled Prediction Interval Estimation of Mechanical Performances for Hot-Rolling Steel. IEEE Transactions on Instrumentation and Measurement, 2022, 71, 1-10.	2.4	5
235	Prospects of Metalâ€Free Perovskites for Piezoelectric Applications. Advanced Science, 2022, 9, e2104703.	5.6	26
236	Machine Learning-Assisted High-Throughput Virtual Screening for On-Demand Customization of Advanced Energetic Materials. Engineering, 2022, 10, 99-109.	3.2	18
237	Evaluation of performance of machine learning methods in mining structureâ€“property data of halide perovskite materials. Chinese Physics B, 2022, 31, 056302.	0.7	8

#	Article	IF	Citations
238	How Machine Learning Predicts and Explains the Performance of Perovskite Solar Cells. Solar Rrl, 2022, 6, .	3.1	26
239	A descriptor for the structural stability of organicâ€“inorganic hybrid perovskites based on binding mechanism in electronic structure. Journal of Molecular Modeling, 2022, 28, 80.	0.8	8
240	Computation of photovoltaic and stability properties of hybrid organicâ€“inorganic perovskites via convolutional neural networks. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	3
241	Accelerated Design of High-Efficiency Lead-Free Tin Perovskite Solar Cells via Machine Learning. International Journal of Precision Engineering and Manufacturing - Green Technology, 2023, 10, 109-121.	2.7	9
242	Machine learning in computational chemistry. Scientia Sinica Chimica, 2022, 52, 858-868.	0.2	2
243	Machine learning accelerated calculation and design of electrocatalysts for CO₂ reduction. SmartMat, 2022, 3, 68-83.	6.4	31
244	Predicting Experimental Formability of Hybrid Organicâ€“Inorganic Perovskites via Imbalanced Learning. Journal of Physical Chemistry Letters, 2022, 13, 3032-3038.	2.1	9
245	Quick screening stable double perovskite oxides for photovoltaic applications by machine learning. Ceramics International, 2022, 48, 18074-18082.	2.3	10
246	How computations accelerate electrocatalyst discovery. CheM, 2022, 8, 1575-1610.	5.8	23
247	Application of deep neural network learning in composites design. European Journal of Materials, 2022, 2, 117-170.	0.8	12
248	Accelerated discovery of high-performance piezocatalyst in BaTiO3-based ceramics via machine learning. Nano Energy, 2022, 97, 107218.	8.2	23
249	Machine learning combined with feature engineering to search for BaTiO3 based ceramics with large piezoelectric constant. Journal of Alloys and Compounds, 2022, 908, 164468.	2.8	14
250	Machine learning based photovoltaic energy prediction scheme by augmentation of on-site IoT data. Future Generation Computer Systems, 2022, 134, 1-12.	4.9	5
251	Probabilistic deep learning approach for targeted hybrid organic-inorganic perovskites. Physical Review Materials, 2021, 5, .	0.9	5
252	Machine learning prediction of 2D perovskite photovoltaics and interaction with energetic ion implantation. Applied Physics Letters, 2021, 119, .	1.5	12
253	Machine Learning-Assisted Development of Organic Solar Cell Materials: Issues, Analyses, and Outlooks. Journal of Physical Chemistry Letters, 2021, 12, 12391-12401.	2.1	38
254	Data-Driven Design of Nanopore Graphene for Water Desalination. Journal of Physical Chemistry C, 2021, 125, 27685-27692.	1.5	12
255	Discovery of Leadâ€Free Perovskites for Highâ€Performance Solar Cells via Machine Learning: Ultrabroadband Absorption, Low Radiative Combination, and Enhanced Thermal Conductivities. Advanced Science, 2022, 9, e2103648.	5.6	35

#	Article	IF	Citations
256	An Ensemble Learning Platform for the Large-Scale Exploration of New Double Perovskites. ACS Applied Materials & Interfaces, 2022, 14, 717-725.	4.0	16
257	Deep machine learning unravels the structural origin of midâ€gap states in chalcogenide glass for highâ€density memory integration. InformaÄnÃ-MateriÃ¡ly, 2022, 4, .	8.5	34
258	Toward Ecoâ€Friendly Leadâ€Free Lowâ€Dimensional Perovskites. Small Structures, 2022, 3, .	6.9	9
259	Dataâ€Driven Materials Innovation and Applications. Advanced Materials, 2022, 34, e2104113.	11.1	51
260	Discovery of Pb-free hybrid organicâ€“inorganic 2D perovskites using a stepwise optimization strategy. Npj Computational Materials, 2022, 8, .	3.5	9
261	Optoelectronic Properties Prediction of Lead-Free Methylammonium Alkaline-Earth Perovskite Based on DFT Calculations. ACS Omega, 2022, 7, 16204-16210.	1.6	6
262	The Electronic Structure of Cs₂AgBiBr₆ at Room Temperature. Physica Status Solidi (B): Basic Research, 2022, 259, .	0.7	13
263	A Machine Learning Framework to Predict the Tensile Stress of Natural Rubber: Based on Molecular Dynamics Simulation Data. Polymers, 2022, 14, 1897.	2.0	3
264	Multi-task graph neural networks for simultaneous prediction of global and atomic properties in ferromagnetic systems [*]. Machine Learning: Science and Technology, 2022, 3, 025007.	2.4	8
265	Machine learning-assisted design of flow fields for redox flow batteries. Energy and Environmental Science, 2022, 15, 2874-2888.	15.6	23
266	ABO3 Perovskitesâ€™ Formability Prediction and Crystal Structure Classification using Machine Learning. , 2022, , .		4
267	Machine learning enabled development of unexplored perovskite solar cells with high efficiency. Nano Energy, 2022, 99, 107394.	8.2	27
268	Machine learning and symbolic regression for adsorption of atmospheric molecules on low-dimensional TiO2. Applied Surface Science, 2022, 597, 153728.	3.1	9
269	High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications. Accounts of Materials Research, 2022, 3, 572-583.	5.9	21
270	Machine-Learning-Assisted Catalytic Performance Predictions of Single-Atom Alloys for Acetylene Semihydrogenation. ACS Applied Materials & Interfaces, 2022, 14, 25288-25296.	4.0	9
271	Accelerated Mining of 2D Van der Waals Heterojunctions by Integrating Supervised and Unsupervised Learning. Chemistry of Materials, 2022, 34, 5571-5583.	3.2	7
272	Exploration of the oxidation and ablation resistance of ultra-high-temperature ceramic coatings using machine learning. Ceramics International, 2022, 48, 28428-28437.	2.3	4
273	Modelling Interfaces in Thin-Film Photovoltaic Devices. Frontiers in Chemistry, 0, 10, .	1.8	3

#	Article	IF	Citations
274	Inorganic Crystal Structure Prototype Database Based on Unsupervised Learning of Local Atomic Environments. Journal of Physical Chemistry A, 0, , .	1.1	1
275	Properties of AgBiI4 using high through-put DFT and machine learning methods. Journal of Applied Physics, 2022, 131, .	1.1	8
276	Inverse Design of Hybrid Organicâ€“Inorganic Perovskites with Suitable Bandgaps via Proactive Searching Progress. ACS Omega, 2022, 7, 21583-21594.	1.6	14
277	â€œSabatier principleâ€•of d electron number for describing the nitrogen reduction reaction performance of single-atom alloy catalysts. Journal of Materials Chemistry A, 2022, 10, 16900-16907.	5.2	22
278	Transition-Metal Interlink Neural Network: Machine Learning of 2D Metalâ€“Organic Frameworks with High Magnetic Anisotropy. ACS Applied Materials & Interfaces, 2022, 14, 33726-33733.	4.0	9
279	Improving Symbolic Regression for Predicting Materials Properties with Iterative Variable Selection. Journal of Chemical Theory and Computation, 2022, 18, 4945-4951.	2.3	11
280	Data-Driven Analysis of Hole-Transporting Materials for Perovskite Solar Cells Performance. Journal of Physical Chemistry C, 2022, 126, 13053-13061.	1.5	13
281	Design of super-hard high-entropy ceramics coatings via machine learning. Ceramics International, 2022, 48, 32064-32072.	2.3	13
282	Interpretable learning of voltage for electrode design of multivalent metal-ion batteries. Npj Computational Materials, 2022, 8, .	3.5	10
283	High-throughput screening of perovskite inspired bismuth halide materials: toward lead-free photovoltaic cells and light-emitting diodes. Nanotechnology, 2022, 33, 485706.	1.3	3
284	Machine learning algorithms in the environmental corrosion evaluation of reinforced concrete structures - A review. Cement and Concrete Composites, 2022, 133, 104725.	4.6	18
285	DeepXRD, a Deep Learning Model for Predicting XRD spectrum from Material Composition. ACS Applied Materials & Interfaces, 2022, 14, 40102-40115.	4.0	8
286	Tunable Dualâ€Band White Light Emission from Gua₃CuCl₄ and Gua₇Cu₃X₁₀Â·3DMF (Xâ€‰=â€‰Br, I). Advanced Photonics Research, 2022, 3, .	2.2	4
287	Machine learning guided phase formation prediction of high entropy alloys. Materials Today Communications, 2022, 32, 104146.	0.9	5
288	Mechanical properties, failure mechanisms, and scaling laws of bicontinuous nanoporous metallic glasses. Acta Materialia, 2022, 239, 118255.	3.8	8
289	Acid-activated Hibiscus sabdariffa seed pods biochar for the adsorption of Chloroquine phosphate: Prediction of adsorption efficiency via machine learning approach.. South African Journal of Chemical Engineering, 2022, 42, 162-175.	1.2	4
290	Accelerated exploration of efficient ternary solar cells with PTB7:PC₇₁BM:SMPV1 using machine-learning methods. Physical Chemistry Chemical Physics, 2022, 24, 22538-22545.	1.3	8
291	Data-driven design of dual-metal-site catalysts for the electrochemical carbon dioxide reduction reaction. Journal of Materials Chemistry A, 2022, 10, 18803-18811.	5.2	14

#	Article	IF	Citations
292	Materials genome engineering-based hydrogen storage materialsdatabase and its applications. Scientia Sinica Chimica, 2022, 52, 1863-1870.	0.2	1
293	Topological feature engineering for machine learning based halide perovskite materials design. Npj Computational Materials, 2022, 8, .	3.5	16
294	Machineâ€Learning Modeling for Ultraâ€Stable Highâ€Efficiency Perovskite Solar Cells. Advanced Energy Materials, 2022, 12, .	10.2	23
295	Applications of machine learning in perovskite materials. Advanced Composites and Hybrid Materials, 2022, 5, 2700-2720.	9.9	43
296	Recent Developments in Process Digitalisation for Advanced Nanomaterial Syntheses. Chemistry Methods, 2022, 2, .	1.8	2
297	Machine Learning for Harnessing Thermal Energy: From Materials Discovery to System Optimization. ACS Energy Letters, 2022, 7, 3204-3226.	8.8	11
298	MetaNOR: A meta-learnt nonlocal operator regression approach for metamaterial modeling. MRS Communications, 2022, 12, 662-677.	0.8	3
299	Accelerated innovation in developing high-performance metal halide perovskite solar cell using machine learning. International Journal of Modern Physics B, 2023, 37, .	1.0	2
300	Prediction of Carbon Dioxide Reduction Catalyst Using Machine Learning with a Few-Feature Model: WLEDZ. Journal of Physical Chemistry C, 2022, 126, 17025-17035.	1.5	7
301	Challenges, Opportunities, and Prospects in Metal Halide Perovskites from Theoretical and Machine Learning Perspectives. Advanced Energy Materials, 2022, 12, .	10.2	19
302	Mapping the Room-Temperature Dynamic Stabilities of Inorganic Halide Double Perovskites. Chemistry of Materials, 2022, 34, 9072-9085.	3.2	2
303	Into the Unknown: How Computation Can Help Explore Uncharted Material Space. Journal of the American Chemical Society, 2022, 144, 18730-18743.	6.6	15
304	Machine learning models for photonic crystals band diagram prediction and gap optimisation. Photonics and Nanostructures - Fundamentals and Applications, 2022, 52, 101076.	1.0	6
305	Stabilized photoemission from organic molecules in zero-dimensional hybrid Zn and Cd halides. Inorganic Chemistry Frontiers, 2022, 9, 6202-6210.	3.0	6
306	Lead-free all-inorganic halide double perovskite materials for optoelectronic applications: progress, performance and design. Physical Chemistry Chemical Physics, 2022, 24, 26948-26961.	1.3	6
307	Machine learning-driven advanced development of carbon-based luminescent nanomaterials. Journal of Materials Chemistry C, 2022, 10, 17431-17450.	2.7	6
308	Scalable training of graph convolutional neural networks for fast and accurate predictions of HOMO-LUMO gap in molecules. Journal of Cheminformatics, 2022, 14, .	2.8	5
309	Machine learning for a sustainable energy future. Nature Reviews Materials, 2023, 8, 202-215.	23.3	76

#	Article	IF	Citations
310	Predicting band gaps and band-edge positions of oxide perovskites using density functional theory and machine learning. Physical Review B, 2022, 106, .	1.1	4
311	Structural screening and descriptor exploration of black phosphorus carbide supported bifunctional catalysts for lithium-sulfur batteries. Journal of Colloid and Interface Science, 2023, 630, 317-327.	5.0	3
312	Theory, properties and engineering of 2D magnetic materials. Progress in Materials Science, 2023, 132, 101036.	16.0	19
313	Data-driven materials discovery and synthesis using machine learning methods. , 2022, , .		0
314	Machine Learning Applications for The TensileÂProperty Evaluation of Steel: An Overview. , 2022, , 1957-1974.		0
315	Compositional engineering of perovskites with machine learning. Physical Review Materials, 2022, 6, .	0.9	4
316	Modulation to favorable surface adsorption energy for oxygen evolution reaction intermediates over carbon-tunable alloys towards sustainable hydrogen production. Materials for Renewable and Sustainable Energy, 2022, 11, 169-213.	1.5	3
317	Openâ€circuit voltage loss and dielectric constants as new descriptors in machine learning study on organic photovoltaics. International Journal of Quantum Chemistry, 0, , .	1.0	2
318	Machine learning-driven design of promising perovskites for photovoltaic applications: A review. Surfaces and Interfaces, 2022, 35, 102470.	1.5	4
319	Machine learning accelerates the materials discovery. Materials Today Communications, 2022, 33, 104900.	0.9	11
320	Review on Perovskite-Type Compound Using Machine Learning. Science of Advanced Materials, 2022, 14, 1001-1017.	0.1	2
321	Optimal design of thermoelectric properties of graphene nanoribbons with 5-7 ring defects based on Bayesian algorithm. Wuli Xuebao/Acta Physica Sinica, 2023, .	0.2	0
322	Accurate property prediction with interpretable machine learning model for small datasets via transformed atom vector. Physical Review Materials, 2022, 6, .	0.9	1
323	A universal training scheme and the resulting universality for machine learning phases. Progress of Theoretical and Experimental Physics, 2023, 2023, .	1.8	3
324	Clearâ€Box Machine Learning for Virtual Screening of 2D Nanozymes to Target Tumor Hydrogen Peroxide. Advanced Healthcare Materials, 2023, 12, .	3.9	8
325	Neural network evidence of a weakly first-order phase transition for the two-dimensional 5-state Potts model. European Physical Journal Plus, 2022, 137, .	1.2	1
327	Machine learning assisted synthetic acceleration of Ruddlesden-Popper and Dion-Jacobson 2D lead halide perovskites. Acta Materialia, 2023, 245, 118638.	3.8	14
328	Perspectives of Machine Learning Development on Kerogen Molecular Model Reconstruction and Shale Oil/Gas Exploitation. Energy & Fuels, 2023, 37, 98-117.	2.5	4

#	Article	IF	Citations
329	Hybrid perovskites under pressure: Present and future directions. Journal of Applied Physics, 2022, 132, .	1.1	4
330	An integrated machine learning model for accurate and robust prediction of superconducting critical temperature. Journal of Energy Chemistry, 2023, 78, 232-239.	7.1	6
331	Bibliometric Analysis of Fourth Industrial Revolution Applied to Material Sciences Based on Web of Science and Scopus Databases from 2017 to 2021. ChemEngineering, 2023, 7, 2.	1.0	8
332	Inâ€Silico Device Performance Prediction of Cosensitizer Dye Pairs for Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2023, 13, .	10.2	1
333	å…‰ç”µåŠŸèƒ½æææ–™çš„ç‡è®ºè®¾è®¡. Chinese Science Bulletin, 2023, , .	0.4	0
334	Recent Advance of Machine Learning in Selecting New Materials. Acta Chimica Sinica, 2023, 81, 158.	0.5	2
335	Thinking green with 2-D and 3-D MXenes: Environment friendly synthesis and industrial scale applications and global impact. Renewable and Sustainable Energy Reviews, 2023, 178, 113238.	8.2	16
336	Efficient discovery of room temperature magnetic transition metal monolayers assisted by artificial neural network. Computational Materials Science, 2023, 224, 112166.	1.4	3
337	Machine learning investigation to predict the relationship between photoluminescence and crystalline properties of blue phosphor Ba0.9-xSrxMgAl10O17:Eu2+. Journal of Science: Advanced Materials and Devices, 2023, 8, 100550.	1.5	1
338	Explaining of prediction accuracy on phase selection of amorphous alloys and high entropy alloys using support vector machines in machine learning. Materials Today Communications, 2023, 35, 105694.	0.9	1
339	High-throughput calculation and machine learning of two-dimensional halide perovskite materials: Formation energy and band gap. Materials Today Communications, 2023, 35, 105841.	0.9	3
340	Understanding the hydrogen evolution reaction activity of doped single-atom catalysts on two-dimensional GaPS4 by DFT and machine learning. Journal of Energy Chemistry, 2023, 81, 93-100.	7.1	17
341	Predicting the HOMO-LUMO gap of benzenoid polycyclic hydrocarbons via interpretable machine learning. Chemical Physics Letters, 2023, 814, 140358.	1.2	6
342	Machine Learning for Perovskite Solar Cells and Component Materials: Key Technologies and Prospects. Advanced Functional Materials, 2023, 33, .	7.8	19
343	Artificial Intelligence Approaches for Energetic Materials by Design: State of the Art, Challenges, and Future Directions. Propellants, Explosives, Pyrotechnics, 2023, 48, .	1.0	3
344	High-throughput screening of hybrid quaternary halide perovskites for optoelectronics. Journal of Materials Chemistry A, 2023, 11, 6465-6473.	5.2	2
345	Enhancing Biochar-Based Nonradical Persulfate Activation Using Data-Driven Techniques. Environmental Science & Technology, 2023, 57, 4050-4059.	4.6	30
346	Identification of potential solid-state Li-ion conductors with semi-supervised learning. Energy and Environmental Science, 2023, 16, 1264-1276.	15.6	5

#	Article	IF	Citations
347	Physicsâ€Based Humanâ€inâ€theâ€Loop Machine Learning Combined with Genetic Algorithm Search for Multicriteria Optimization: Electrochemical CO₂ Reduction Reaction. Advanced Intelligent Systems, 2023, 5, .	3.3	1
348	Exploring the relationship between lattice distortion and phase stability in a multi-principal element alloy system based on machine learning method. Computational Materials Science, 2023, 221, 112089.	1.4	9
349	Machine Learning in Unmanned Systems for Chemical Synthesis. Molecules, 2023, 28, 2232.	1.7	2
350	Predicting Sulfurâ€Rich Oxysulfide Perovskites for Waterâ€Splitting Applications Using Machine Learning. Advanced Theory and Simulations, 2023, 6, .	1.3	2
351	Targetâ€Driven Design of Deepâ€UV Nonlinear Optical Materials via Interpretable Machine Learning. Advanced Materials, 2023, 35, .	11.1	18
352	Optimized synthesis of the anti-COVID-19 drugs aided by retrosynthesis software. RSC Medicinal Chemistry, 0, , .	1.7	0
353	Machine-learning-assisted discovery of boron-doped graphene with high work function as an anode material for Li/Na/K-ion batteries. Physical Chemistry Chemical Physics, 2023, 25, 12200-12206.	1.3	2
354	Adaptive Design of Alloys for CO₂ Activation and Methanation via Reinforcement Learning Monte Carlo Tree Search Algorithm. Journal of Physical Chemistry Letters, 2023, 14, 3594-3601.	2.1	1
355	Substitution engineering of lead-free halide perovskites for photocatalytic applications assisted by machine learning. Physical Chemistry Chemical Physics, 2023, 25, 12450-12457.	1.3	1
356	Feature Selection in Machine Learning for Perovskite Materials Design and Discovery. Materials, 2023, 16, 3134.	1.3	6
357	Advances in machine learning- and artificial intelligence-assisted material design of steels. International Journal of Minerals, Metallurgy and Materials, 2023, 30, 1003-1024.	2.4	14
362	AI for Nanomaterials Development in Clean Energy and Carbon Capture, Utilization and Storage (CCUS). ACS Nano, 2023, 17, 9763-9792.	7.3	5
372	The Application of Novel Functional Materials to Machine Learning. , 2023, , 95-115.		0
373	Perovskite-Based Materials for Photovoltaic Applications: A Machine Learning Approach. , 2023, , 139-162.		0
380	Metal Oxide Classification Based on SVM. Lecture Notes in Computer Science, 2023, , 685-694.	1.0	0
382	Critical role of 1D materials in realizing efficient and stable perovskite solar cells. Journal of Materials Chemistry A, 2023, 11, 18592-18604.	5.2	4