

Machine Learning for Chemical Reactions

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Lattice oxygen redox chemistry in solid-state electrocatalysts for water oxidation. <i>Energy and Environmental Science</i> , 2021, 14, 4647-4671.	30.8	190
2	Perspective on integrating machine learning into computational chemistry and materials science. <i>Journal of Chemical Physics</i> , 2021, 154, 230903.	3.0	107
3	Genesis of Polyatomic Molecules in Dark Clouds: CO ₂ Formation on Cold Amorphous Solid Water. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6781-6787.	4.6	7
4	Applying Machine Learning to Rechargeable Batteries: From the Microscale to the Macroscale. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24354-24366.	13.8	67
5	Applying Machine Learning to Rechargeable Batteries: From the Microscale to the Macroscale. <i>Angewandte Chemie</i> , 2021, 133, 24558-24570.	2.0	11
6	Automated Exploration of Prebiotic Chemical Reaction Space: Progress and Perspectives. <i>Life</i> , 2021, 11, 1140.	2.4	6
7	Transfer learned potential energy surfaces: accurate anharmonic vibrational dynamics and dissociation energies for the formic acid monomer and dimer. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5269-5281.	2.8	15
8	Machine Learning of Reaction Properties via Learned Representations of the Condensed Graph of Reaction. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2101-2110.	5.4	48
9	Opportunities and challenges of organic flow battery for electrochemical energy storage technology. <i>Journal of Energy Chemistry</i> , 2022, 67, 621-639.	12.9	39
10	Theoretical Studies on Triplet-state Driven Dissociation of Formaldehyde by Quasi-classical Molecular Dynamics Simulation on Machine-Learning Potential Energy Surface. <i>Journal of Chemical Physics</i> , 2021, 155, 214105.	3.0	3
11	Automated Construction of Neural Network Potential Energy Surface: The Enhanced Self-Organizing Incremental Neural Network Deep Potential Method. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5425-5437.	5.4	6
12	A new permutation-symmetry-adapted machine learning diabatisation procedure and its application in MgH ₂ system. <i>Journal of Chemical Physics</i> , 2021, 155, 214102.	3.0	5
13	Gradient domain machine learning with composite kernels: improving the accuracy of PES and force fields for large molecules. <i>Machine Learning: Science and Technology</i> , 2022, 3, 015005.	5.0	4
14	Predicting trajectory behaviour via machine-learned invariant manifolds. <i>Chemical Physics Letters</i> , 2022, 789, 139290.	2.6	2
15	Machine learning product state distributions from initial reactant states for a reactive atom-diatom collision system. <i>Journal of Chemical Physics</i> , 2022, 156, 034301.	3.0	10
16	Uncertainty-aware prediction of chemical reaction yields with graph neural networks. <i>Journal of Cheminformatics</i> , 2022, 14, 2.	6.1	17
17	Potential Application of Machine-Learning-Based Quantum Chemical Methods in Environmental Chemistry. <i>Environmental Science & Technology</i> , 2022, 56, 2115-2123.	10.0	22
18	Towards artificial intelligence at scale in the chemical industry. <i>AIChE Journal</i> , 2022, 68, .	3.6	12

#	ARTICLE	IF	CITATIONS
19	Providing direction for mechanistic inferences in radical cascade cyclization using a Transformer model. <i>Organic Chemistry Frontiers</i> , 2022, 9, 2498-2508.	4.5	6
20	SPA ^H M: the spectrum of approximated Hamiltonian matrices representations. , 2022, 1, 286-294.		7
21	Influence of second-order saddles on reaction mechanisms. <i>Faraday Discussions</i> , 0, , .	3.2	2
22	Interpretable Machine Learning for Investigating Photoelectrochemical Properties of Cosensitizer-Based CH ₃ NH ₃ PbI ₃ /TiO ₂ Films in Water. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6482-6490.	3.1	9
23	Photodissociation dynamics of N ₃ ⁺ . <i>Journal of Chemical Physics</i> , 2022, 156, 124307.	3.0	0
24	Atomistic Simulations for Reactions and Vibrational Spectroscopy in the Era of Machine Learning” <i>Quo Vadis?</i> . <i>Journal of Physical Chemistry B</i> , 2022, 126, 2155-2167.	2.6	8
25	Towards Predictive Synthesis of Inorganic Materials Using Network Science. <i>Frontiers in Chemistry</i> , 2021, 9, 798838.	3.6	2
26	Ring-Polymer Molecular Dynamics Calculations of Thermal Rate Coefficients and Branching Ratios for the Interstellar H ₃ ⁺ + CO → H ₂ + HCO ⁺ /HOC ⁺ Reaction and Its Deuterated Analogue. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10750-10756.	2.5	6
27	On the Cartesian Representation of the Molecular Polarizability Tensor Surface by Polynomial Fitting to <i>Ab Initio</i> Data. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 37-45.	5.3	4
28	Quantitative molecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12767-12786.	2.8	3
29	Double proton transfer in hydrated formic acid dimer: Interplay of spatial symmetry and solvent-generated force on reactivity. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13869-13882.	2.8	7
30	Quantum Gaussian process model of potential energy surface for a polyatomic molecule. <i>Journal of Chemical Physics</i> , 2022, 156, 184802.	3.0	3
31	Applying Classical, <i>Ab Initio</i> , and Machine-Learning Molecular Dynamics Simulations to the Liquid Electrolyte for Rechargeable Batteries. <i>Chemical Reviews</i> , 2022, 122, 10970-11021.	47.7	138
32	Low-cost prediction of molecular and transition state partition functions <i>via</i> machine learning. <i>Chemical Science</i> , 2022, 13, 7900-7906.	7.4	4
33	Combined QM/MM, Machine Learning Path Integral Approach to Compute Free Energy Profiles and Kinetic Isotope Effects in RNA Cleavage Reactions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4304-4317.	5.3	17
34	Fast Predictions of Reaction Barrier Heights: Toward Coupled-Cluster Accuracy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3976-3986.	2.5	26
35	Efficient and Accurate Description of Diels-Alder Reactions Using Density Functional Theory**. <i>ChemPhysChem</i> , 2022, 23, .	2.1	6
36	Mechanistic Inference from Statistical Models at Different Data-Size Regimes. <i>ACS Catalysis</i> , 2022, 12, 7886-7906.	11.2	12

#	ARTICLE	IF	CITATIONS
37	Machine learning analysis of dynamicâ€dependent bond formation in trajectories with consecutive transition states. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	1.9	8
38	Applying neural network force field on water nucleation. , 2022, , .		0
39	The Use of Machine Learning Model in the Evaluation of College Studentsâ€™ Employment and Entrepreneurship Level. <i>Wireless Communications and Mobile Computing</i> , 2022, 2022, 1-10.	1.2	5
40	Progress of Experimental and Computational Catalyst Design for Electrochemical Nitrogen Fixation. <i>ACS Catalysis</i> , 2022, 12, 8936-8975.	11.2	41
41	Review of Machine Learning for Hydrodynamics, Transport, and Reactions in Multiphase Flows and Reactors. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 9901-9949.	3.7	63
42	Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. <i>Chemical Reviews</i> , 2022, 122, 13478-13515.	47.7	120
43	Machine Learning Modeling of Environmentally Relevant Chemical Reactions for Organic Compounds. <i>ACS ES&T Water</i> , 2024, 4, 773-783.	4.6	8
44	Highâ€throughput Screening of Bicationic Redox Materials for Chemical Looping Ammonia Synthesis. <i>Advanced Science</i> , 2022, 9, .	11.2	7
45	Machine Learning Predicts the X-ray Photoelectron Spectroscopy of the Solid Electrolyte Interface of Lithium Metal Battery. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 8047-8054.	4.6	16
46	Neural network potentials. , 2023, , 279-294.		1
47	Machine Learning for Efficient Prediction of Protein Redox Potential: The Flavoproteins Case. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4748-4759.	5.4	5
48	Automatic Evolution of Machine-Learning-Based Quantum Dynamics with Uncertainty Analysis. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5837-5855.	5.3	6
49	Uncertainty quantification for predictions of atomistic neural networks. <i>Chemical Science</i> , 2022, 13, 13068-13084.	7.4	7
50	Towards fully ab initio simulation of atmospheric aerosol nucleation. <i>Nature Communications</i> , 2022, 13, .	12.8	6
51	SELFIES and the future of molecular string representations. <i>Patterns</i> , 2022, 3, 100588.	5.9	49
52	A systematic literature review for the prediction of anticancer drug response using various machineâ€learning and deepâ€learning techniques. <i>Chemical Biology and Drug Design</i> , 2023, 101, 175-194.	3.2	6
53	Computational design of magnetic molecules and their environment using quantum chemistry, machine learning and multiscale simulations. <i>Nature Reviews Chemistry</i> , 2022, 6, 761-781.	30.2	21
54	Controlled Synthesis of Multicolor Carbon Dots Assisted by Machine Learning. <i>Advanced Functional Materials</i> , 2023, 33, .	14.9	16

#	ARTICLE	IF	CITATIONS
55	Chemical transformations and transport phenomena at interfaces. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	5
56	Multi-scale modeling of crystal-fluid interactions: State-of-the-art, challenges and prospects. , 2024, , 760-792.		1
57	Molecular Dynamics with Conformationally Dependent, Distributed Charges. Journal of Chemical Theory and Computation, 0, , .	5.3	2
58	Atomistic neural network representations for chemical dynamics simulations of molecular, condensed phase, and interfacial systems: Efficiency, representability, and generalization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	11
59	Toward autonomous laboratories: Convergence of artificial intelligence and experimental automation. Progress in Materials Science, 2023, 132, 101043.	32.8	19
60	High-dimensional neural network potentials for accurate vibrational frequencies: the formic acid dimer benchmark. Physical Chemistry Chemical Physics, 2022, 24, 29381-29392.	2.8	7
61	Neural network potentials for chemistry: concepts, applications and prospects. , 2023, 2, 28-58.		17
62	Machine learning for the yield prediction of CO ₂ cyclization reaction catalyzed by the ionic liquids. Fuel, 2023, 335, 126942.	6.4	1
63	Sustainability in Wood Products: A New Perspective for Handling Natural Diversity. Chemical Reviews, 2023, 123, 1889-1924.	47.7	15
64	Novel Lennard-Jones Parameters for Cysteine and Selenocysteine in the AMBER Force Field. Journal of Chemical Information and Modeling, 2023, 63, 595-604.	5.4	3
65	Benchmarking general neural network potential $\langle \text{ANI} \rangle_{\text{ax}}$ on aerosol nucleation molecular clusters. International Journal of Quantum Chemistry, 2023, 123, .	2.0	3
66	Artificial intelligence models for yield efficiency optimization, prediction, and production scalability of essential oil extraction processes from citrus fruit exocarps. Frontiers in Chemical Engineering, 0, 4, .	2.7	0
67	Electron Microscopy Studies of Soft Nanomaterials. Chemical Reviews, 2023, 123, 4051-4145.	47.7	16
68	Chemical reaction networks and opportunities for machine learning. Nature Computational Science, 2023, 3, 12-24.	8.0	16
69	HTE and machine learning-assisted development of iridium($\langle \text{i} \rangle$)-catalyzed selective O-H bond insertion reactions toward carboxymethyl ketones. Organic Chemistry Frontiers, 2023, 10, 1153-1159.	4.5	5
70	Machine learning based implicit solvent model for aqueous-solution alanine dipeptide molecular dynamics simulations. RSC Advances, 2023, 13, 4565-4577.	3.6	5
72	Explainable uncertainty quantifications for deep learning-based molecular property prediction. Journal of Cheminformatics, 2023, 15, .	6.1	10
73	Drug discovery: Standing on the shoulders of giants. , 2023, , 207-338.		0

#	ARTICLE	IF	CITATIONS
74	Machine learning assisted advanced battery thermal management system: A state-of-the-art review. <i>Journal of Energy Storage</i> , 2023, 60, 106688.	8.1	12
75	Machine Learning and Deep Learning Promote Computational Toxicology for Risk Assessment of Chemicals. <i>Computational Methods in Engineering & the Sciences</i> , 2023, , 1-17.	0.3	1
76	Overview on Theoretical Simulations of Lithium-Ion Batteries and Their Application to Battery Separators. <i>Advanced Energy Materials</i> , 2023, 13, .	19.5	29
77	Progress of Artificial Intelligence in Drug Synthesis and Prospect of Its Application in Nitrification of Energetic Materials. <i>Molecules</i> , 2023, 28, 1900.	3.8	0
78	How Beneficial or Threatening is Artificial Intelligence?. <i>Chem-Bio Informatics Journal</i> , 2023, 23, 7-13.	0.3	0
79	Rationalizing Functionalized MXenes as Effective Anchor Materials for Lithium-Sulfur Batteries via First-Principles Calculations. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2215-2221.	4.6	4
80	MLRNet: Combining the Physics-Motivated Potential Models with Neural Networks for Intermolecular Potential Energy Surface Construction. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1421-1431.	5.3	1
81	Machine Learning Assisted Simulations of Electrochemical Interfaces: Recent Progress and Challenges. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 2308-2316.	4.6	9
82	Retrosynthesis from transforms to predictive sustainable chemistry and nanotechnology: a brief tutorial review. <i>Green Chemistry</i> , 2023, 25, 2971-2991.	9.0	3
83	ESTIMATING FORMATION MECHANISM OF DISINFECTION BY-PRODUCTS AND MOLECULAR COMPOSITIONS OF THEIR PRECURSOR NOM USING ULTRA-HIGH RESOLUTION MASS SPECTROMETRY. <i>Journal of Japan Society of Civil Engineers Ser G (Environmental Research)</i> , 2022, 78, III_185-III_194.	0.1	0
84	Combining Machine Learning with Physical Knowledge in Thermodynamic Modeling of Fluid Mixtures. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2023, 14, 31-51.	6.8	9
85	Perovskite oxide composites for bifunctional oxygen electrocatalytic activity and zinc-air battery application- a mini-review. <i>Energy Storage Materials</i> , 2023, 58, 362-380.	18.0	12
86	Combustion, Chemistry, and Carbon Neutrality. <i>Chemical Reviews</i> , 2023, 123, 5139-5219.	47.7	37
87	Machine learning in energy chemistry: introduction, challenges and perspectives. <i>Energy Advances</i> , 2023, 2, 896-921.	3.3	6
88	Analyzing drop coalescence in microfluidic devices with a deep learning generative model. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 15744-15755.	2.8	1
89	Machine learning and analytical methods for single-molecule conductance measurements. <i>Chemical Communications</i> , 2023, 59, 6796-6810.	4.1	3
90	Perspective: Reference-Potential Methods for the Study of Thermodynamic Properties in Chemical Processes: Theory, Applications, and Pitfalls. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 4866-4875.	4.6	2
91	Data-driven design of new chiral carboxylic acid for construction of indoles with C-central and C ^α -N axial chirality via cobalt catalysis. <i>Nature Communications</i> , 2023, 14, .	12.8	8

#	ARTICLE	IF	CITATIONS
92	pyCHARMM: Embedding CHARMM Functionality in a Python Framework. Journal of Chemical Theory and Computation, 2023, 19, 3752-3762.	5.3	5
93	Matrix of orthogonalized atomic orbital coefficients representation for radicals and ions. Journal of Chemical Physics, 2023, 158, .	3.0	3
94	Learning Organotransition Metal Reactions Using Graph Neural Networks. Journal of Computer Chemistry Japan, 2022, 21, 126-128.	0.1	0
95	Molecular dynamics for electrocatalysis: Mechanism explanation and performance prediction. , 2023, 2, 100028.		6
96	Manipulating hydrogen bond dissociation rates and mechanisms in water dimer through vibrational strong coupling. Nature Communications, 2023, 14, .	12.8	5
97	Machine Learning-Directed Predictive Models: Deciphering Complex Energy Transfer in Mn-Doped CsPb(Cl _{1-x} Br ₃) Perovskite Nanocrystals. Chemistry of Materials, 2023, 35, 5401-5411.	6.7	3
98	Efficient interatomic descriptors for accurate machine learning force fields of extended molecules. Nature Communications, 2023, 14, .	12.8	2
99	Faster Response Chemical Reaction Using Machine Learning. , 2023, , .		0
100	Enhanced Copolymer Characterization for Polyethers Using Gel Permeation Chromatography Combined with Artificial Neural Networks. Analytical Chemistry, 2023, 95, 10504-10511.	6.5	2
101	Halide Vacancies Create No Charge Traps on Lead Halide Perovskite Surfaces but Can Generate Deep Traps in the Bulk. Journal of Physical Chemistry Letters, 2023, 14, 6028-6036.	4.6	8
102	High-Throughput Condensed-Phase Hybrid Density Functional Theory for Large-Scale Finite-Gap Systems: The SeA Approach. Journal of Chemical Theory and Computation, 2023, 19, 4182-4201.	5.3	2
103	Unsupervised Analysis of Optical Imaging Data for the Discovery of Reactivity Patterns in Metal Alloy. Small Methods, 2023, 7, .	8.6	5
104	Reaction mechanism “ explored with the unified reaction valley approach. Chemical Communications, 2023, 59, 7151-7165.	4.1	0
105	Recent Advances in Machine Learning for Electrochemical, Optical, and Gas Sensors. , 2023, , 117-138.		0
106	Challenges for Kinetics Predictions via Neural Network Potentials: A Wilkinson’s Catalyst Case. Molecules, 2023, 28, 4477.	3.8	0
107	Transfer-learned potential energy surfaces: Toward microsecond-scale molecular dynamics simulations in the gas phase at CCSD(T) quality. Journal of Chemical Physics, 2023, 158, .	3.0	4
108	Parametrically Managed Activation Function for Fitting a Neural Network Potential with Physical Behavior Enforced by a Low-Dimensional Potential. Journal of Physical Chemistry A, 2023, 127, 5287-5297.	2.5	2
109	Machine Learning for Bridging the Gap between Density Functional Theory and Coupled Cluster Energies. Journal of Chemical Theory and Computation, 2023, 19, 4912-4920.	5.3	1

#	ARTICLE	IF	CITATIONS
110	PhysNet meets CHARMM: A framework for routine machine learning/molecular mechanics simulations. Journal of Chemical Physics, 2023, 159, .	3.0	3
112	Exploiting machine learning for controlled synthesis of carbon dots-based corrosion inhibitors. Journal of Cleaner Production, 2023, 419, 138210.	9.3	15
113	Applications of machine learning in supercritical fluids research. Journal of Supercritical Fluids, 2023, 202, 106051.	3.2	4
114	Prediction of product distribution using machine learning techniques. Computer Aided Chemical Engineering, 2023, , 673-678.	0.5	0
115	Unlocking the Potential: Predicting Redox Behavior of Organic Molecules, from Linear Fits to Neural Networks. Journal of Chemical Theory and Computation, 2023, 19, 4796-4814.	5.3	1
116	Open-Source Machine Learning in Computational Chemistry. Journal of Chemical Information and Modeling, 2023, 63, 4505-4532.	5.4	3
117	Developing machine learning approaches to identify candidate persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances based on molecular structure. Water Research, 2023, 244, 120470.	11.3	3
118	"Freedom of Design" in Chemical Compound Space: Towards Rational <i>in Silico</i> Design of Molecules with Targeted Quantum-Mechanical Properties. Chemical Science, 0, , .	7.4	0
119	Reactant-induced dynamics of lithium imide surfaces during the ammonia decomposition process. Nature Catalysis, 2023, 6, 829-836.	34.4	9
120	Thermodynamic and kinetic modeling of electrocatalytic reactions using a first-principles approach. Journal of Chemical Physics, 2023, 159, .	3.0	0
121	Emerging Two-Dimensional Organic Semiconductor-Incorporated Perovskitesâ€”A Fascinating Family of Hybrid Electronic Materials. Journal of the American Chemical Society, 2023, 145, 20694-20715.	13.7	5
122	Comment on â€”Physics-based representations for machine learning properties of chemical reactionsâ€” TM . Machine Learning: Science and Technology, 2023, 4, 048001.	5.0	1
123	Photodynamics With Neural Networks and Kernel Ridge Regression. , 2024, , 413-426.		0
124	Machine Learning-Assisted Low-Dimensional Electrocatalysts Design for Hydrogen Evolution Reaction. Nano-Micro Letters, 2023, 15, .	27.0	7
125	Applications and Advances in Machine Learning Force Fields. Journal of Chemical Information and Modeling, 0, , .	5.4	0
126	Reformulating Reactivity Design for Data-Efficient Machine Learning. ACS Catalysis, 2023, 13, 13506-13515.	11.2	1
127	Zeolite encapsulated organometallic complexes as model catalysts. Dalton Transactions, 0, , .	3.3	0
128	Machine Learning-Based Analysis of Molar and Enantiomeric Ratios and Reaction Yields Using Images of Solid Mixtures. Industrial & Engineering Chemistry Research, 2023, 62, 13790-13798.	3.7	0

#	ARTICLE	IF	CITATIONS
129	Deep learning-assisted calculation of apparent activation energy for cement-based systems incorporating microencapsulated phase change materials. <i>Construction and Building Materials</i> , 2023, 404, 133324.	7.2	1
130	Application of non-local mean image denoising algorithm based on machine learning technology in visual communication design. <i>Journal of Intelligent and Fuzzy Systems</i> , 2023, , 1-13.	1.4	0
131	An improved artificial neural network fit of the ab initio potential energy surface points for HeH ⁺ + H ₂ and its ensuing rigid rotors quantum dynamics. , 2023, 1, 100017.		0
133	Learning organo- π -transition metal catalyzed reactions by graph neural networks. <i>Journal of Computational Chemistry</i> , 0, , .	3.3	0
134	Molecular simulation approaches to study crystal nucleation from solutions: Theoretical considerations and computational challenges. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2024, 14, .	14.6	1
135	High-Dimensional Neural Network Potentials for Accurate Prediction of Equation of State: A Case Study of Methane. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 7825-7832.	5.3	0
136	Thermal conversion potential of tea stems: Experimental investigation, reaction mechanism, and kinetic modeling. <i>Industrial Crops and Products</i> , 2024, 207, 117753.	5.2	0
137	An explainability framework for deep learning on chemical reactions exemplified by enzyme-catalysed reaction classification. <i>Journal of Cheminformatics</i> , 2023, 15, .	6.1	0
138	Transfer learning for a foundational chemistry model. <i>Chemical Science</i> , 0, , .	7.4	1
139	Fast prediction and control of air core in hydrocyclone by machine learning to stabilize operations. <i>Journal of Environmental Chemical Engineering</i> , 2024, 12, 111699.	6.7	1
140	Enabling late-stage drug diversification by high-throughput experimentation with geometric deep learning. <i>Nature Chemistry</i> , 2024, 16, 239-248.	13.6	1
141	A machine learning approach for predicting the reactivity power of hypervalent iodine compounds. , 2024, 2, 100032.		0
142	Accelerated Chemical Science with AI. , 0, , .		0
143	Effects of Aleatoric and Epistemic Errors in Reference Data on the Learnability and Quality of NN-based Potential Energy Surfaces. , 2023, , 100033.		0
144	Accurate fundamental invariant-neural network representation of <i>ab initio</i> potential energy surfaces. <i>National Science Review</i> , 0, , .	9.5	4
145	Effluent quality prediction of the sewage treatment based on a hybrid neural network model: Comparison and application. <i>Journal of Environmental Management</i> , 2024, 351, 119900.	7.8	0
146	Harvesting Chemical Understanding with Machine Learning and Quantum Computers. <i>ACS Physical Chemistry Au</i> , 2024, 4, 135-142.	4.0	0
147	Generating a skeleton reaction network for reactions of large-scale ReaxFF MD pyrolysis simulations based on a machine learning predicted reaction class. <i>Physical Chemistry Chemical Physics</i> , 2024, 26, 5649-5668.	2.8	0

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148	Reaction Space Charting as a Tool in Organic Chemistry Research and Development. <i>Advanced Synthesis and Catalysis</i> , 2024, 366, 551-573.	4.3	0
149	Applying graph neural network models to molecular property prediction using high-quality experimental data. , 2024, 2, 100050.		0
150	Scientific Deep Machine Learning Concepts for the Prediction of Concentration Profiles and Chemical Reaction Kinetics: Consideration of Reaction Conditions. <i>Journal of Physical Chemistry A</i> , 2024, 128, 929-944.	2.5	0
151	Life cycle analysis of hydrogen production from aqueous phase reforming of glycerol. <i>International Journal of Hydrogen Energy</i> , 2024, , .	7.1	0
152	Mixtures Recomposition by Neural Nets: A Multidisciplinary Overview. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 597-620.	5.4	1
153	Machine learning prediction of state-to-state rate constants for astrochemistry. , 2024, 2, 100052.		0
154	Molecular Contrastive Pretraining with Collaborative Featurizations. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 1112-1122.	5.4	0
155	Comparative Analysis of Shallow Learning and Deep Learning. , 2023, , .		0
156	Surface-Accelerated String Method for Locating Minimum Free Energy Paths. <i>Journal of Chemical Theory and Computation</i> , 2024, 20, 2058-2073.	5.3	0
157	Recent Developments in Machine Learning for Mass Spectrometry. <i>ACS Measurement Science Au</i> , 0, , .	4.4	0
158	Prediction of chemical reaction yields with large-scale multi-view pre-training. <i>Journal of Cheminformatics</i> , 2024, 16, .	6.1	0
159	Improving chemical reaction yield prediction using pre-trained graph neural networks. <i>Journal of Cheminformatics</i> , 2024, 16, .	6.1	0
160	Artificial molecular pumps. <i>Nature Reviews Methods Primers</i> , 2024, 4, .	21.2	0
161	Machine Learning Isotropic $\langle i \rangle_g \langle i \rangle$ Values of Radical Polymers. <i>Journal of Chemical Theory and Computation</i> , 2024, 20, 2592-2604.	5.3	0
162	Decoding Electrochemical Processes of Lithium-Ion Batteries by Classical Molecular Dynamics Simulations. <i>Advanced Energy Materials</i> , 0, , .	19.5	0
164	Probe into the volumetric properties of binary mixtures: Essence of regression-based machine learning algorithms. <i>Journal of Molecular Liquids</i> , 2024, 399, 124498.	4.9	0
165	A globally accurate neural network potential energy surface and quantum dynamics study of $\text{Mg}^+(2\text{S})\text{A}^+\text{H}_2\text{A}^+\text{MgH}^+ + \text{H}$ reaction. <i>Chemical Physics Letters</i> , 2024, 842, 141223.	2.6	0
166	Numerical Accuracy Matters: Applications of Machine Learned Potential Energy Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2024, 15, 3419-3424.	4.6	0