

Deep-learning-based inverse design model for intelligent

Npj Computational Materials

4,

DOI: [10.1038/s41524-018-0128-1](https://doi.org/10.1038/s41524-018-0128-1)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Nanoinformatics, and the big challenges for the science of small things. <i>Nanoscale</i> , 2019, 11, 19190-19201.	2.8	59
2	Machine learning in materials science. <i>InformaĀnĀ-MateriĀly</i> , 2019, 1, 338-358.	8.5	427
3	Convolutional Neural Networks for the Design and Analysis of Non-Fullerene Acceptors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4993-5001.	2.5	29
4	Virtual Issue on Machine-Learning Discoveries in Materials Science. <i>Chemistry of Materials</i> , 2019, 31, 8243-8247.	3.2	23
5	A property-oriented design strategy for high performance copper alloys via machine learning. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	104
6	Deep Learning to Generate <i>in Silico</i> Chemical Property Libraries and Candidate Molecules for Small Molecule Identification in Complex Samples. <i>Analytical Chemistry</i> , 2020, 92, 1720-1729.	3.2	62
7	InverseĀQSPR for <i>de novo</i> Design: A Review. <i>Molecular Informatics</i> , 2020, 39, e1900087.	1.4	27
8	Deep-Learning Architecture in QSPR Modeling for the Prediction of Energy Conversion Efficiency of Solar Cells. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 18991-19000.	1.8	13
9	Dirty engineering data-driven inverse prediction machine learning model. <i>Scientific Reports</i> , 2020, 10, 20443.	1.6	9
10	Who Is Metabolizing What? Discovering Novel Biomolecules in the Microbiome and the Organisms Who Make Them. <i>Frontiers in Cellular and Infection Microbiology</i> , 2020, 10, 388.	1.8	6
11	EvoMol: a flexible and interpretable evolutionary algorithm for unbiased <i>de novo</i> molecular generation. <i>Journal of Cheminformatics</i> , 2020, 12, 55.	2.8	29
12	Smart Manufacturing for Smart CitiesĀOverview, Insights, and Future Directions. <i>Advanced Intelligent Systems</i> , 2020, 2, 2000043.	3.3	29
13	Machine-Learning-Assisted <i>De Novo</i> Design of Organic Molecules and Polymers: Opportunities and Challenges. <i>Polymers</i> , 2020, 12, 163.	2.0	95
14	Machine learning in experimental materials chemistry. <i>Catalysis Today</i> , 2021, 371, 77-84.	2.2	36
15	<i>De novo</i> generation of optically active small organic molecules using Monte Carlo tree search combined with recurrent neural network. <i>Journal of Computational Chemistry</i> , 2021, 42, 136-143.	1.5	8
16	Data-driven algorithms for inverse design of polymers. <i>Soft Matter</i> , 2021, 17, 7607-7622.	1.2	39
17	Deep learning-enabled prediction of 2D material breakdown. <i>Nanotechnology</i> , 2021, 32, 265203.	1.3	6
19	Predicting Infrared Spectra with Message Passing Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2594-2609.	2.5	31

#	ARTICLE	IF	CITATIONS
20	Quantum Chemistry Calculations for Metabolomics. <i>Chemical Reviews</i> , 2021, 121, 5633-5670.	23.0	47
22	Active-Learning-Based Generative Design for the Discovery of Wide-Band-Gap Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 16118-16128.	1.5	12
23	Evolutionary design of molecules based on deep learning and a genetic algorithm. <i>Scientific Reports</i> , 2021, 11, 17304.	1.6	19
24	Deep learning framework for material design space exploration using active transfer learning and data augmentation. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	70
25	Recent machine learning guided material research - A review. <i>Computational Condensed Matter</i> , 2021, 29, e00597.	0.9	4
26	Tackling the Challenge of a Huge Materials Science Search Space with Quantum-Inspired Annealing. <i>Advanced Intelligent Systems</i> , 2021, 3, 2000209.	3.3	15
27	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13557-13583.	2.7	20
28	Discovery of Lead-Free Hybrid Organic/Inorganic Perovskites Using Metaheuristic-Driven DFT Calculations. <i>Chemistry of Materials</i> , 2021, 33, 782-798.	3.2	23
29	Generative Models for Automatic Chemical Design. <i>Lecture Notes in Physics</i> , 2020, , 445-467.	0.3	42
30	Deep learning and generative methods in cheminformatics and chemical biology: navigating small molecule space intelligently. <i>Biochemical Journal</i> , 2020, 477, 4559-4580.	1.7	29
31	Forward and inverse design of kirigami via supervised autoencoder. <i>Physical Review Research</i> , 2020, 2, .	1.3	39
32	Machine Learning in Materials Discovery: Confirmed Predictions and Their Underlying Approaches. <i>Annual Review of Materials Research</i> , 2020, 50, 49-69.	4.3	75
33	DeepReac+: deep active learning for quantitative modeling of organic chemical reactions. <i>Chemical Science</i> , 2021, 12, 14459-14472.	3.7	20
34	MolGPT: Molecular Generation Using a Transformer-Decoder Model. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2064-2076.	2.5	105
35	Convolutional neural networks for the design and analysis of nonfullerene acceptors. , 2022, , 231-256.		25
36	Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.		0
37	Bayesian optimization for chemical products and functional materials. <i>Current Opinion in Chemical Engineering</i> , 2022, 36, 100728.	3.8	43
38	De Novo Molecular Design with Chemical Language Models. <i>Methods in Molecular Biology</i> , 2022, 2390, 207-232.	0.4	3

#	ARTICLE	IF	CITATIONS
39	Deep learning approaches for de novo drug design: An overview. <i>Current Opinion in Structural Biology</i> , 2022, 72, 135-144.	2.6	54
40	Decoding hexanitrobenzene (HNB) and 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) as two distinctive energetic nitrobenzene compounds by machine learning. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9875-9884.	1.3	12
41	Inverse Design of Materials by Machine Learning. <i>Materials</i> , 2022, 15, 1811.	1.3	28
42	Effect of molecular representation on deep learning performance for prediction of molecular electronic properties. <i>Bulletin of the Korean Chemical Society</i> , 0, , .	1.0	1
43	Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation. <i>Frontiers in Materials</i> , 2022, 9, .	1.2	19
44	Artificial intelligence to bring nanomedicine to life. <i>Advanced Drug Delivery Reviews</i> , 2022, 184, 114194.	6.6	39
45	Two-dimensional finite element network analysis: Formulation and static analysis of structural assemblies. <i>Computers and Structures</i> , 2022, 266, 106784.	2.4	2
46	Artificial intelligence: machine learning for chemical sciences. <i>Journal of Chemical Sciences</i> , 2022, 134, 2.	0.7	32
47	Virtual Screening for Organic Solar Cells and Light Emitting Diodes. <i>Advanced Science</i> , 2022, 9, e2200825.	5.6	13
48	Accelerated Discovery of the Polymer Blends for Cartilage Repair through Data-Mining Tools and Machine-Learning Algorithm. <i>Polymers</i> , 2022, 14, 1802.	2.0	5
49	Evaluation of Deep Learning Architectures for Aqueous Solubility Prediction. <i>ACS Omega</i> , 2022, 7, 15695-15710.	1.6	20
50	Efficient Adversarial Generation of Thermally Activated Delayed Fluorescence Molecules. <i>ACS Omega</i> , 2022, 7, 18179-18188.	1.6	5
51	Deep learning approaches for <i>de novo</i> drug design: an overview. <i>Scientia Sinica Chimica</i> , 2023, 53, 95-106.	0.2	2
52	MACAW: An Accessible Tool for Molecular Embedding and Inverse Molecular Design. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3551-3564.	2.5	4
53	UV-Visible Absorption Spectra of Solvated Molecules by Quantum Chemical Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4891-4902.	2.3	6
54	Machine learning-assisted evaluation of potential biochars for pharmaceutical removal from water. <i>Environmental Research</i> , 2022, 214, 113953.	3.7	10
55	Inverse design of nanophotonic devices using generative adversarial networks. <i>Engineering Applications of Artificial Intelligence</i> , 2022, 115, 105259.	4.3	7
56	Bandgap prediction on small thermoelectric material dataset via instance-based transfer learning. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113872.	1.1	3

#	ARTICLE	IF	CITATIONS
57	Transformation rule-based molecular evolution for automatic gasoline molecule design. <i>Chemical Engineering Science</i> , 2022, 263, 118119.	1.9	1
58	OGGN: A Novel Generalized Oracle Guided Generative Architecture for Modelling Inverse Function of Artificial Neural Networks. <i>Communications in Computer and Information Science</i> , 2022, , 460-471.	0.4	0
59	Efficient enumeration-selection computational strategy for adaptive chemistry. <i>Scientific Reports</i> , 2022, 12, .	1.6	0
60	QCforever: A Quantum Chemistry Wrapper for Everyone to Use in Black-Box Optimization. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4427-4434.	2.5	4
61	Methodology for the design of the emissive Ir complex with the ab-initio screening and the reinforcement learning. , 2022, , .		0
62	Data-driven materials discovery and synthesis using machine learning methods. , 2022, , .		0
63	Roles and opportunities for machine learning in organic molecular crystal structure prediction and its applications. <i>MRS Bulletin</i> , 2022, 47, 1054-1062.	1.7	3
64	Dynamic Modeling of Intrinsic Self-Healing Polymers Using Deep Learning. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 52486-52498.	4.0	2
65	Electronic, redox, and optical property prediction of organic π -conjugated molecules through a hierarchy of machine learning approaches. <i>Chemical Science</i> , 2022, 14, 203-213.	3.7	4
66	Computational Design and Manufacturing of Sustainable Materials through First-Principles and Materiomics. <i>Chemical Reviews</i> , 2023, 123, 2242-2275.	23.0	16
67	Physics-informed machine learning combining experiment and simulation for the design of neodymium-iron-boron permanent magnets with reduced critical-elements content. <i>Frontiers in Materials</i> , 0, 9, .	1.2	10
68	MatFlow: A System for Knowledge-based Novel Materials Design using Machine Learning. , 2022, , .		0
69	High-throughput transient photoluminescence spectrometer for deep learning of thermally activated delayed fluorescence materials. <i>Journal of Materials Chemistry C</i> , 2023, 11, 4357-4364.	2.7	2
70	Convolved filtering for process cycle modeling. <i>Engineering Reports</i> , 2023, 5, .	0.9	2
71	Predicting power conversion efficiency of binary organic solar cells based on Y6 acceptor by machine learning. <i>Journal of Energy Chemistry</i> , 2023, 82, 139-147.	7.1	7
72	TEXplorer.org: Thermoelectric material properties data platform for experimental and first-principles calculation results. <i>APL Materials</i> , 2023, 11, .	2.2	4
73	Computational Approaches for Organic Semiconductors: From Chemical and Physical Understanding to Predicting New Materials. <i>Chemical Reviews</i> , 2023, 123, 7498-7547.	23.0	11