Logan Ward

List of Publications by Year
in descending order

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51 papers	3,580 citations	331670 21 h-index	276875 41 g-index
55 all docs	55 docs citations	55 times ranked	3478 citing authors

#	Article	IF	Citations
1	A general-purpose machine learning framework for predicting properties of inorganic materials. Npj Computational Materials, 2016, 2, .	8.7	922
2	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
3	Accelerated discovery of metallic glasses through iteration of machine learning and high-throughput experiments. Science Advances, 2018, 4, eaaq1566.	10.3	354
4	Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations. Physical Review B, 2017, 96, .	3.2	254
5	ElemNet: Deep Learning the Chemistry of Materials From Only Elemental Composition. Scientific Reports, 2018, 8, 17593.	3.3	242
6	Atomistic calculations and materials informatics: A review. Current Opinion in Solid State and Materials Science, 2017, 21, 167-176.	11.5	169
7	A machine learning approach for engineering bulk metallic glass alloys. Acta Materialia, 2018, 159, 102-111.	7.9	163
8	Can machine learning identify the next high-temperature superconductor? Examining extrapolation performance for materials discovery. Molecular Systems Design and Engineering, 2018, 3, 819-825.	3.4	149
9	A data ecosystem to support machine learning in materials science. MRS Communications, 2019, 9, 1125-1133.	1.8	112
10	Structural evolution and kinetics in Cu-Zr metallic liquids from molecular dynamics simulations. Physical Review B, 2013, 88, .	3.2	85
11	Machine-learning-accelerated high-throughput materials screening: Discovery of novel quaternary Heusler compounds. Physical Review Materials, 2018, 2, .	2.4	62
12	Feature engineering for machine learning enabled early prediction of battery lifetime. Journal of Power Sources, 2022, 527, 231127.	7.8	43
13	The <scp>MolSSI</scp> QCA<scp>rchive</scp> project: An openâ€source platform to compute, organize, and share quantum chemistry data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1491.	14.6	42
14	Machine learning prediction of accurate atomization energies of organic molecules from low-fidelity quantum chemical calculations. MRS Communications, 2019, 9, 891-899.	1.8	38
15	DLHub: Model and Data Serving for Science. , 2019, , .		36
16	A High-Throughput Structural and Electrochemical Study of Metallic Glass Formation in Niâ€“Tiâ€“Al. ACS Combinatorial Science, 2020, 22, 330-338.	3.8	31
17	Simulation of discrete damage in composite Overheight Compact Tension specimens. Composites Part A: Applied Science and Manufacturing, 2012, 43, 1667-1679.	7.6	30
18	Strategies for accelerating the adoption of materials informatics. MRS Bulletin, 2018, 43, 683-689.	3.5	29

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19	Enabling deeper learning on big data for materials informatics applications. Scientific Reports, 2021, 11, 4244.	3.3	29
20	Quantum-Chemically Informed Machine Learning: Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms. Journal of Physical Chemistry A, 2020, 124, 5804-5811.	2.5	28
21	Automated Development of Molten Salt Machine Learning Potentials: Application to LiCl. Journal of Physical Chemistry Letters, 2021, 12, 4278-4285.	4.6	26
22	IRNet. , 2019, , .		23
23	Design Strategy for High-Performance Thermoelectric Materials: The Prediction of Electron-Doped KZrCuSe₃. Chemistry of Materials, 2019, 31, 3018-3024.	6.7	23
24	Dataâ€driven glass/ceramic science research: Insights from the glass and ceramic and data science/informatics communities. Journal of the American Ceramic Society, 2019, 102, 6385-6406.	3.8	20
25	Colmena: Scalable Machine-Learning-Based Steering of Ensemble Simulations for High Performance Computing. , 2021, , .		20
26	An embedded atom method potential of beryllium. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 085001.	2.0	18
27	DLHub: Simplifying publication, discovery, and use of machine learning models in science. Journal of Parallel and Distributed Computing, 2021, 147, 64-76.	4.1	17
28	Ternary mixed-anion semiconductors with tunable band gaps from machine-learning and crystal structure prediction. Physical Review Materials, 2019, 3, .	2.4	16
29	Automated crystal structure solution from powder diffraction data: Validation of the first-principles-assisted structure solution method. Physical Review Materials, 2017, 1, .	2.4	15
30	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
31	Discovering exceptionally hard and wear-resistant metallic glasses by combining machine-learning with high throughput experimentation. Applied Physics Reviews, 2022, 9, .	11.3	12
32	Serverless Workflows for Indexing Large Scientific Data. , 2019, , .		11
33	High-throughput crystal structure solution using prototypes. Physical Review Materials, 2021, 5, .	2.4	11
34	Challenges and Advances in Information Extraction from Scientific Literature: a Review. Jom, 2021, 73, 3383-3400.	1.9	11
35	Graph-Based Approaches for Predicting Solvation Energy in Multiple Solvents: Open Datasets and Machine Learning Models. Journal of Physical Chemistry A, 2021, 125, 5990-5998.	2.5	10
36	Fundamental Insights from a Singleâ€Crystal Sodium Iridate Battery. Advanced Energy Materials, 2020, 10, 1903128.	19.5	9

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37	Machine Learning Prediction of the Critical Cooling Rate for Metallic Glasses from Expanded Datasets and Elemental Features. Chemistry of Materials, 2022, 34, 2945-2954.	6.7	9
38	Data automation at light sources. AIP Conference Proceedings, 2019, , .	0.4	8
39	Active Learning Yields Better Training Data for Scientific Named Entity Recognition. , 2019, , .		7
40	Co-design Center for Exascale Machine Learning Technologies (ExaLearn). International Journal of High Performance Computing Applications, 2021, 35, 598-616.	3.7	6
41	Proxima. , 2021, , .		5
42	The structure of Cuâ€“Zr glasses using a colloidal proxy system. Acta Materialia, 2013, 61, 2025-2032.	7.9	4
43	Three new crystal structures in the Naâ€“Pb system: solving structures without additional experimental input. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, 542-548.	0.1	4
44	Towards hybrid human-machine scientific information extraction. , 2018, , .		4
45	Publishing and Serving Machine Learning Models with DLHub. , 2019, , .		4
46	Structural property comparison of Caâ€“Mgâ€“Zn glasses to a colloidal proxy system. Acta Materialia, 2013, 61, 6911-6917.	7.9	3
47	Improving the Accuracy of Composite Methods: A G4MP2 Method with G4-like Accuracy and Implications for Machine Learning. Journal of Physical Chemistry A, 2022, 126, 4528-4536.	2.5	3
48	Models and Processes to Extract Drug-like Molecules From Natural Language Text. Frontiers in Molecular Biosciences, 2021, 8, 636077.	3.5	1
49	First-Principles-Assisted Structure Solution: Leveraging Density Functional Theory to Solve Experimentally Observed Crystal Structures. , 2019, , 1-14.		0
50	Development of new Mg-Zn-Sr alloys for medical purpose. International Journal of Nanotechnology, 2020, 17, 573.	0.2	0
51	First-Principles-Assisted Structure Solution: Leveraging Density Functional Theory to Solve Experimentally Observed Crystal Structures. , 2020, , 2835-2848.		0