Rohit Batra

List of Publications by Year
in descending order

38 papers	3,691 citations	257450 24 h-index	330143 37 g-index
39 all docs	39 docs citations	39 times ranked	4001 citing authors

#	Article	IF	Citations
1	Machine learning in materials informatics: recent applications and prospects. Npj Computational Materials, 2017, 3, .	8.7	1,013
2	Machine Learning Force Fields: Construction, Validation, and Outlook. Journal of Physical Chemistry C, 2017, 121, 511-522.	3.1	368
3	Solving the electronic structure problem with machine learning. Npj Computational Materials, 2019, 5, .	8.7	191
4	A universal strategy for the creation of machine learning-based atomistic force fields. Npj Computational Materials, 2017, 3, .	8.7	188
5	PhysicallyÂinformed artificial neural networks for atomistic modeling of materials. Nature Communications, 2019, 10, 2339.	12.8	177
6	Factors Favoring Ferroelectricity in Hafnia: A First-Principles Computational Study. Journal of Physical Chemistry C, 2017, 121, 4139-4145.	3.1	158
7	Dopants Promoting Ferroelectricity in Hafnia: Insights from a comprehensive Chemical Space Exploration. Chemistry of Materials, 2017, 29, 9102-9109.	6.7	139
8	Emerging materials intelligence ecosystems propelled by machine learning. Nature Reviews Materials, 2021, 6, 655-678.	48.7	138
9	Polymer informatics: Current status and critical next steps. Materials Science and Engineering Reports, 2021, 144, 100595.	31.8	117
10	Machine-learning predictions of polymer properties with Polymer Genome. Journal of Applied Physics, 2020, 128, .	2.5	111
11	Stabilization of metastable phases in hafnia owing to surface energy effects. Applied Physics Letters, 2016, 108, .	3.3	108
12	Polymer design using genetic algorithm and machine learning. Computational Materials Science, 2021, 186, 110067.	3.0	105
13	Prediction of water stability of metalâ€“organic frameworks using machine learning. Nature Machine Intelligence, 2020, 2, 704-710.	16.0	89
14	Machine learning models for the lattice thermal conductivity prediction of inorganic materials. Computational Materials Science, 2019, 170, 109155.	3.0	84
15	Electrochemical Stability Window of Polymeric Electrolytes. Chemistry of Materials, 2019, 31, 4598-4604.	6.7	83
16	Screening of Therapeutic Agents for COVID-19 Using Machine Learning and Ensemble Docking Studies. Journal of Physical Chemistry Letters, 2020, 11, 7058-7065.	4.6	82
17	Frequency-dependent dielectric constant prediction of polymers using machine learning. Npj Computational Materials, 2020, 6, .	8.7	75
18	Multifidelity Information Fusion with Machine Learning: A Case Study of Dopant Formation Energies in Hafnia. ACS Applied Materials & Interfaces, 2019, 11, 24906-24918.	8.0	49

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19	A multi-fidelity information-fusion approach to machine learn and predict polymer bandgap. Computational Materials Science, 2020, 172, 109286.	3.0	49
20	Polymers for Extreme Conditions Designed Using Syntax-Directed Variational Autoencoders. Chemistry of Materials, 2020, 32, 10489-10500.	6.7	43
21	Predicting Crystallization Tendency of Polymers Using Multifidelity Information Fusion and Machine Learning. Journal of Physical Chemistry B, 2020, 124, 6046-6054.	2.6	35
22	General Atomic Neighborhood Fingerprint for Machine Learning-Based Methods. Journal of Physical Chemistry C, 2019, 123, 15859-15866.	3.1	33
23	Accurate machine learning in materials science facilitated by using diverse data sources. Nature, 2021, 589, 524-525.	27.8	29
24	Electronic Structure of Polymer Dielectrics: The Role of Chemical and Morphological Complexity. Chemistry of Materials, 2018, 30, 7699-7706.	6.7	26
25	Artificial Intelligence-Guided De Novo Molecular Design Targeting COVID-19. ACS Omega, 2021, 6, 12557-12566.	3.5	22
26	Learning in continuous action space for developing high dimensional potential energy models. Nature Communications, 2022, 13, 368.	12.8	21
27	Iterative-Learning Strategy for the Development of Application-Specific Atomistic Force Fields. Journal of Physical Chemistry C, 2019, 123, 20715-20722.	3.1	20
28	Refractive index prediction models for polymers using machine learning. Journal of Applied Physics, 2020, 127, .	2.5	20
29	Machine learning models for the prediction of energy, forces, and stresses for Platinum. Computational Materials Science, 2020, 174, 109483.	3.0	17
30	A charge density prediction model for hydrocarbons using deep neural networks. Machine Learning: Science and Technology, 2020, 1, 025003.	5.0	15
31	Crystal Morphology and Phase Transformation of LiAlO₂: Combined Experimental and First-Principles Studies. Journal of Physical Chemistry C, 2018, 122, 28797-28804.	3.1	14
32	Thermodynamics of Phase Stability and Ferroelectricity From First Principles. , 2019, , 245-289.		13
33	Learning with Delayed Rewardsâ€"A Case Study on Inverse Defect Design in 2D Materials. ACS Applied Materials & Interfaces, 2021, 13, 36455-36464.	8.0	12
34	Machine learning for multi-fidelity scale bridging and dynamical simulations of materials. JPhys Materials, 2020, 3, 031002.	4.2	11
35	A comprehensive computational study of adatom diffusion on the aluminum (1â€¯0â€¯0) surface. Computational Materials Science, 2019, 158, 353-358.	3.0	9
36	Search for Ferroelectric Binary Oxides: Chemical and Structural Space Exploration Guided by Group Theory and Computations. Chemistry of Materials, 2020, 32, 3823-3832.	6.7	9

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37	Multi-reward Reinforcement Learning Based Bond-Order Potential to Study Strain-Assisted Phase Transitions in Phosphorene. Journal of Physical Chemistry Letters, 2022, 13, 1886-1893.	4.6	9
38	Machine learning the metastable phase diagram of covalently bonded carbon. Nature Communications, 2022, 13, .	12.8	9