Kamal Choudhary

List of Publications by Year
in descending order

66 papers	2,541 citations	236612 25 h-index	197535 49 g-index
67 all docs	67 docs citations	67 times ranked	2924 citing authors

#	Article	IF	Citations
1	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	3.5	207
2	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
3	High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory. Scientific Reports, 2017, 7, 5179.	1.6	173
4	Enhancing materials property prediction by leveraging computational and experimental data using deep transfer learning. Nature Communications, 2019, 10, 5316.	5.8	160
5	Atomistic Line Graph Neural Network for improved materials property predictions. Npj Computational Materials, 2021, 7, .	3.5	159
6	Characterization of Few-Layer 1Tâ€² MoTe$_2$ by Polarization-Resolved Second Harmonic Generation and Raman Scattering. ACS Nano, 2016, 10, 9626-9636.	7.3	148
7	Materials science in the artificial intelligence age: high-throughput library generation, machine learning, and a pathway from correlations to the underpinning physics. MRS Communications, 2019, 9, 821-838.	0.8	109
8	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	1.4	95
9	Machine learning with force-field-inspired descriptors for materials: Fast screening and mapping energy landscape. Physical Review Materials, 2018, 2, .	0.9	90
10	Elastic properties of bulk and low-dimensional materials using van der Waals density functional. Physical Review B, 2018, 98, .	1.1	88
11	Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods. Chemistry of Materials, 2019, 31, 5900-5908.	3.2	87
12	Computational screening of high-performance optoelectronic materials using OptB88vdW and TB-mBJ formalisms. Scientific Data, 2018, 5, 180082.	2.4	79
13	Convergence and machine learning predictions of Monkhorst-Pack k-points and plane-wave cut-off in high-throughput DFT calculations. Computational Materials Science, 2019, 161, 300-308.	1.4	68
14	High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses. Npj Computational Materials, 2020, 6, .	3.5	60
15	Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data. Nature Communications, 2021, 12, 6595.	5.8	55
16	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
17	Computational Discovery of Inorganic Electrides from an Automated Screening. Matter, 2019, 1, 1293-1303.	5.0	42
18	Data-driven discovery of 3D and 2D thermoelectric materials. Journal of Physics Condensed Matter, 2020, 32, 475501.	0.7	42

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19	Graphene–Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	4.0	37
20	A simple constrained machine learning model for predicting high-pressure-hydrogen-compressor materials. Molecular Systems Design and Engineering, 2018, 3, 509-517.	1.7	37
21	High-throughput Discovery of Topologically Non-trivial Materials using Spin-orbit Spillage. Scientific Reports, 2019, 9, 8534.	1.6	36
22	Computational search for magnetic and non-magnetic 2D topological materials using unified spin–orbit spillage screening. Npj Computational Materials, 2020, 6, .	3.5	32
23	Artificial intelligence for search and discovery of quantum materials. Communications Materials, 2021, 2, .	2.9	29
24	Probing the accuracy of reactive and non-reactive force fields to describe physical and chemical properties of graphene-oxide. Computational Materials Science, 2016, 114, 236-243.	1.4	26
25	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
26	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
27	Klein-Gordon equation approach to nonlinear split-ring resonator based metamaterials: One-dimensional systems. Physical Review B, 2011, 84, .	1.1	22
28	High-throughput search for magnetic topological materials using spin-orbit spillage, machine learning, and experiments. Physical Review B, 2021, 103, .	1.1	22
29	Uncertainty Prediction for Machine Learning Models of Material Properties. ACS Omega, 2021, 6, 32431-32440.	1.6	21
30	Database of Wannier tight-binding Hamiltonians using high-throughput density functional theory. Scientific Data, 2021, 8, 106.	2.4	20
31	Graph neural network predictions of metal organic framework CO_2 adsorption properties. Computational Materials Science, 2022, 210, 111388.	1.4	19
32	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. Scientific Data, 2017, 4, 160125.	2.4	18
33	Charge optimized many-body (COMB) potential for Al_2O_3 materials, interfaces, and nanostructures. Journal of Physics Condensed Matter, 2015, 27, 305004.	0.7	17
34	Thermodynamic analysis of the topologically close packed σ phase in the Co Cr system. Intermetallics, 2019, 105, 13-20.	1.8	17
35	Prediction of the Electron Density of States for Crystalline Compounds with Atomistic Line Graph Neural Networks (ALIGNN). Jom, 2022, 74, 1395-1405.	0.9	17
36	Cu cluster deposition on ZnO $(10\bar{1}0)$: Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014,	0.8	16

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37	Computational scanning tunneling microscope image database. Scientific Data, 2021, 8, 57.	2.4	15
38	Fano resonance due to discrete breather in nonlinear Klein–Gordon lattice in metamaterials. Journal of the Optical Society of America B: Optical Physics, 2012, 29, 2414.	0.9	14
39	Discrete breathers in nonlinear LiNbO3-type ferroelectrics. Journal of Applied Physics, 2011, 109, 054105.	1.1	13
40	High-throughput assessment of vacancy formation and surface energies of materials using classical force-fields. Journal of Physics Condensed Matter, 2018, 30, 395901.	0.7	12
41	Quantum pinning-transition due to charge defects in ferroelectrics. Journal of Applied Physics, 2011, 110, 024104.	1.1	11
42	Discrete energy levels of bright solitons in lithium niobate ferroelectrics. Physical Review B, 2012, 86, .	1.1	11
43	An Inter-Laboratory Study of Zn–Sn–Ti–O Thin Films using High-Throughput Experimental Methods. ACS Combinatorial Science, 2019, 21, 350-361.	3.8	11
44	Density functional theory-based electric field gradient database. Scientific Data, 2020, 7, 362.	2.4	11
45	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. Applied Physics Letters, 2015, 107, 112109.	1.5	10
46	Predicting anomalous quantum confinement effect in van der Waals materials. Physical Review Materials, 2021, 5, .	0.9	10
47	Temperature-driven band inversion in $Pb_{1-x}Sn_{x}$... Optical and Hall effect studies. Physical Review B, 2014, 90, .	1.1	9
48	Charge optimized many-body (COMB) potential for dynamical simulation of Ni–Al phases. Journal of Physics Condensed Matter, 2015, 27, 336302.	0.7	8
49	Spin-exchange interaction between transition metals and metalloids in soft-ferromagnetic metallic glasses. Journal of Physics Condensed Matter, 2016, 28, 216003.	0.7	8
50	Efficiently searching extreme mechanical properties via boundless objective-free exploration and minimal first-principles calculations. Npj Computational Materials, 2022, 8, .	3.5	8
51	Charge optimized many-body potential for aluminum. Journal of Physics Condensed Matter, 2015, 27, 015003.	0.7	7
52	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. MRS Advances, 2018, 3, 457-462.	0.5	7
53	Candidate replacements for lead in CH3NH3PbI3 from first principles calculations. Computational Materials Science, 2018, 155, 69-73.	1.4	7
54	Quantum breathers in Klein-Gordon lattice: Non-periodic boundary condition approach. Journal of Applied Physics, 2011, 110, 124106.	1.1	6

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55	Machine learning approaches for feature engineering of the crystal structure: Application to the prediction of the formation energy of cubic compounds. Physical Review Materials, 2021, 5, .	0.9	6
56	Role of coupling of discrete breathers in split-ring-resonator-based metamaterials. Physica Scripta, 2012, 86, 015601.	1.2	5
57	Bound to unbound state route and propagation of dark solitons showing acoustical memory. AIP Advances, 2014, 4, 087101.	0.6	5
58	Quantum computation for predicting electron and phonon properties of solids. Journal of Physics Condensed Matter, 2021, 33, 385501.	0.7	5
59	Machine learning predicted magnetic entropy change using chemical descriptors across a large compositional landscape. Computational Materials Science, 2022, 209, 111414.	1.4	5
60	Discovery and characterization of 2D materials and their heterostructures. , 2020, , 1-11.		4
61	Rectification of energy transport in nonlinear metamaterials via ratchets. Journal Physics D: Applied Physics, 2013, 46, 205102.	1.3	3
62	Atomic-Scale Quantification of the Chemical Modification of Polystyrene through S, SC, and SH Deposition from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 12103-12110.	1.5	1
63	Large scale dataset of real space electronic charge density of cubic inorganic materials from density functional theory (DFT) calculations. Scientific Data, 2022, 9, 59.	2.4	1
64	Quantum breathers in lithium tantalate ferroelectrics. Applied Nanoscience (Switzerland), 2013, 3, 343-355.	1.6	0
65	Mechanisms for hyperthermal polyatomic hydrocarbon modification of PMMA surfaces from molecular dynamics simulations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, 061403.	0.9	0
66	Domain Wall Width in Different Ferroelectrics via Perturbation Route. World Journal of Condensed Matter Physics, 2012, 02, 91-95.	1.1	0