Kamal Choudhary

List of Publications by Year
in descending order

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66	2,541	236612	197535
papers	citations	25 h-index	49 g-index

67	67	67	2924
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	3.5	207
4	Machine learning predicted magnetic entropy change using chemical descriptors across a large compositional landscape. Computational Materials Science, 2022, 209, 111414.	1.4	5
5	Graph neural network predictions of metal organic framework CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e488" altimg="si38.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> adsorption properties. Computational Materials Science, 2022, 210, 111388.	1.4	19
6	Efficiently searching extreme mechanical properties via boundless objective-free exploration and minimal first-principles calculations. Npj Computational Materials, 2022, 8, .	3.5	8
7	Computational scanning tunneling microscope image database. Scientific Data, 2021, 8, 57.	2.4	15
8	High-throughput search for magnetic topological materials using spin-orbit spillage, machine learning, and experiments. Physical Review B, 2021, 103, .	1.1	22
9	Database of Wannier tight-binding Hamiltonians using high-throughput density functional theory. Scientific Data, 2021, 8, 106.	2.4	20
10	Predicting anomalous quantum confinement effect in van der Waals materials. Physical Review Materials, 2021, 5, .	0.9	10
11	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
12	Quantum computation for predicting electron and phonon properties of solids. Journal of Physics Condensed Matter, 2021, 33, 385501.	0.7	5
13	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
14	Artificial intelligence for search and discovery of quantum materials. Communications Materials, 2021, 2, .	2.9	29
15	Uncertainty Prediction for Machine Learning Models of Material Properties. ACS Omega, 2021, 6, 32431-32440.	1.6	21
16	Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data. Nature Communications, 2021, 12, 6595.	5.8	55
17	Atomistic Line Graph Neural Network for improved materials property predictions. Npj Computational Materials, 2021, 7, .	3.5	159
18	Discovery and characterization of 2D materials and their heterostructures. , 2020, , 1-11.		4

#	Article	IF	Citations
19	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
20	Density functional theory-based electric field gradient database. Scientific Data, 2020, 7, 362.	2.4	11
21	Computational search for magnetic and non-magnetic 2D topological materials using unified spinâ€“orbit spillage screening. Npj Computational Materials, 2020, 6, .	3.5	32
22	High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses. Npj Computational Materials, 2020, 6, .	3.5	60
23	Data-driven discovery of 3D and 2D thermoelectric materials. Journal of Physics Condensed Matter, 2020, 32, 475501.	0.7	42
24	Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods. Chemistry of Materials, 2019, 31, 5900-5908.	3.2	87
25	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
26	Computational Discovery of Inorganic Electrides from an Automated Screening. Matter, 2019, 1, 1293-1303.	5.0	42
27	High-throughput Discovery of Topologically Non-trivial Materials using Spin-orbit Spillage. Scientific Reports, 2019, 9, 8534.	1.6	36
28	An Inter-Laboratory Study of Znâ€“Snâ€“Tiâ€“O Thin Films using High-Throughput Experimental Methods. ACS Combinatorial Science, 2019, 21, 350-361.	3.8	11
29	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
30	Enhancing materials property prediction by leveraging computational and experimental data using deep transfer learning. Nature Communications, 2019, 10, 5316.	5.8	160
31	Thermodynamic analysis of the topologically close packed Ïƒ phase in the Co Cr system. Intermetallics, 2019, 105, 13-20.	1.8	17
32	Titanium-Carbide Formation at Defective Curved Graphene-Titanium Interfaces. MRS Advances, 2018, 3, 457-462.	0.5	7
33	Computational screening of high-performance optoelectronic materials using OptB88vdW and TB-mBJ formalisms. Scientific Data, 2018, 5, 180082.	2.4	79
34	Elastic properties of bulk and low-dimensional materials using van der Waals density functional. Physical Review B, 2018, 98, .	1.1	88
35	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
36	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

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37	Candidate replacements for lead in CH3NH3PbI3 from first principles calculations. Computational Materials Science, 2018, 155, 69-73.	1.4	7
38	Machine learning with force-field-inspired descriptors for materials: Fast screening and mapping energy landscape. Physical Review Materials, 2018, 2, .	0.9	90
39	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. Scientific Data, 2017, 4, 160125.	2.4	18
40	Grapheneâ€“Titanium Interfaces from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 33288-33297.	4.0	37
41	High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory. Scientific Reports, 2017, 7, 5179.	1.6	173
42	Spin-exchange interaction between transition metals and metalloids in soft-ferromagnetic metallic glasses. Journal of Physics Condensed Matter, 2016, 28, 216003.	0.7	8
43	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
44	Characterization of Few-Layer 1Tâ€² MoTe₂ by Polarization-Resolved Second Harmonic Generation and Raman Scattering. ACS Nano, 2016, 10, 9626-9636.	7.3	148
45	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
46	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
47	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
48	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. Applied Physics Letters, 2015, 107, 112109.	1.5	10
49	Charge optimized many-body potential for aluminum. Journal of Physics Condensed Matter, 2015, 27, 015003.	0.7	7
50	Charge optimized many-body (COMB) potential for dynamical simulation of Niâ€“Al phases. Journal of Physics Condensed Matter, 2015, 27, 336302.	0.7	8
51	Charge optimized many-body (COMB) potential for Al₂O₃materials, interfaces, and nanostructures. Journal of Physics Condensed Matter, 2015, 27, 305004.	0.7	17
52	Temperature-driven band inversion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pb</mml:mi><mml:mrow><mml:mn>0.77</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Se: Optical and Hall effect studies. Physical Review B, 2014, 90, .	1.1	9
53	"><mml:mfenced open="(" close=")"><mml:mrow><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo stretchy="true">Â¯</mml:mo></mml:mover><mml:mn>0</mml:mn></mml:mrow></mml:mfenced></mml:math>: Morphology and growth mode predicted from molecular dynamics simulations. Surface Science, 2014,	0.8	16
54	Bound to unbound state route and propagation of dark solitons showing acoustical memory. AIP Advances, 2014, 4, 087101.	0.6	5

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55	Quantum breathers in lithium tantalate ferroelectrics. Applied Nanoscience (Switzerland), 2013, 3, 343-355.	1.6	0
56	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
57	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
58	Rectification of energy transport in nonlinear metamaterials via ratchets. Journal Physics D: Applied Physics, 2013, 46, 205102.	1.3	3
59	Fano resonance due to discrete breather in nonlinear Kleinâ€“Gordon lattice in metamaterials. Journal of the Optical Society of America B: Optical Physics, 2012, 29, 2414.	0.9	14
60	Role of coupling of discrete breathers in split-ring-resonator-based metamaterials. Physica Scripta, 2012, 86, 015601.	1.2	5
61	Discrete energy levels of bright solitons in lithium niobate ferroelectrics. Physical Review B, 2012, 86, .	1.1	11
62	Domain Wall Width in Different Ferroelectrics via Perturbation Route. World Journal of Condensed Matter Physics, 2012, 02, 91-95.	1.1	0
63	Klein-Gordon equation approach to nonlinear split-ring resonator based metamaterials: One-dimensional systems. Physical Review B, 2011, 84, .	1.1	22
64	Quantum pinning-transition due to charge defects in ferroelectrics. Journal of Applied Physics, 2011, 110, 024104.	1.1	11
65	Discrete breathers in nonlinear LiNbO3-type ferroelectrics. Journal of Applied Physics, 2011, 109, 054105.	1.1	13
66	Quantum breathers in Klein-Gordon lattice: Non-periodic boundary condition approach. Journal of Applied Physics, 2011, 110, 124106.	1.1	6