Anubhav Jain

List of Publications by Year
in descending order

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110 papers	24,615 citations	34105 52 h-index	27406 106 g-index
124 all docs	124 docs citations	124 times ranked	20894 citing authors

#	Article	IF	Citations
1	Thermal fluids with high specific heat capacity through reversible Diels-Alder reactions. IScience, 2022, 25, 103540.	4.1	2
2	Toward a Mechanistic Model of Solidâ€“Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. ACS Energy Letters, 2022, 7, 1446-1453.	17.4	46
3	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	8.7	207
4	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science. Patterns, 2022, 3, 100488.	5.9	46
5	Text-mined dataset of gold nanoparticle synthesis procedures, morphologies, and size entities. Scientific Data, 2022, 9, .	5.3	24
6	Photovoltaic module antireflection coating degradation survey using color microscopy and spectral reflectance. Progress in Photovoltaics: Research and Applications, 2022, 30, 1270-1288.	8.1	3
7	Automated defect identification in electroluminescence images of solar modules. Solar Energy, 2022, 242, 20-29.	6.1	18
8	Experimental validation of high thermoelectric performance in RECuZnP2 predicted by high-throughput DFT calculations. Materials Horizons, 2021, 8, 209-215.	12.2	38
9	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
10	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31
11	Phase-Transition-Enhanced Thermoelectric Transport in Rickardite Mineral Cu_{3â€“x}Te₂. Chemistry of Materials, 2021, 33, 1832-1841.	6.7	9
12	A simple model for the entropy of melting of monatomic liquids. Applied Physics Letters, 2021, 118, .	3.3	6
13	Optimal band structure for thermoelectrics with realistic scattering and bands. Npj Computational Materials, 2021, 7, .	8.7	25
14	IFermi: A python library for Fermi surface generation and analysis. Journal of Open Source Software, 2021, 6, 3089.	4.6	26
15	Efficient calculation of carrier scattering rates from first principles. Nature Communications, 2021, 12, 2222.	12.8	205
16	Nondestructive Characterization of Antireflective Coatings on PV Modules. IEEE Journal of Photovoltaics, 2021, 11, 760-769.	2.5	7
17	Compromise between band structure and phonon scattering in efficient n-Mg3Sb2-Bi thermoelectrics. Materials Today Physics, 2021, 18, 100362.	6.0	41
18	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	13.6	240

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19	When band convergence is not beneficial for thermoelectrics. Nature Communications, 2021, 12, 3425.	12.8	51
20	A framework for quantifying uncertainty in DFT energy corrections. Scientific Reports, 2021, 11, 15496.	3.3	51
21	Insight into SEI Growth in Li-Ion Batteries using Molecular Dynamics and Accelerated Chemical Reactions. Journal of Physical Chemistry C, 2021, 125, 18588-18596.	3.1	24
22	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
23	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
24	Reducing Interanalyst Variability in Photovoltaic Degradation Rate Assessments. IEEE Journal of Photovoltaics, 2020, 10, 206-212.	2.5	22
25	Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of Na₃V₂(PO₄)₂F₃. Chemistry of Materials, 2020, 32, 8981-8992.	6.7	14
26	Gapped metals as thermoelectric materials revealed by high-throughput screening. Journal of Materials Chemistry A, 2020, 8, 17579-17594.	10.3	19
27	Benchmarking materials property prediction methods: the Matbench test set and Automatminer reference algorithm. Npj Computational Materials, 2020, 6, .	8.7	96
28	A critical examination of compound stability predictions from machine-learned formation energies. Npj Computational Materials, 2020, 6, .	8.7	119
29	High Thermoelectric Performance and Defect Energetics of Multipocketed Full Heusler Compounds. Physical Review Applied, 2020, 14, .	3.8	25
30	Computational discovery of promising new n-type dopable ABX Zintl thermoelectric materials. Materials Horizons, 2020, 7, 1809-1818.	12.2	30
31	An automatically curated first-principles database of ferroelectrics. Scientific Data, 2020, 7, 72.	5.3	39
32	Aqueous Dielsâ€“Alder reactions for thermochemical storage and heat transfer fluids identified using density functional theory. Journal of Computational Chemistry, 2020, 41, 2137-2150.	3.3	4
33	Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity. RSC Advances, 2020, 10, 6063-6081.	3.6	57
34	Photovoltaic String Sizing Using Site-Specific Modeling. IEEE Journal of Photovoltaics, 2020, 10, 888-897.	2.5	5
35	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
36	Machine Learning Chemical Guidelines for Engineering Electronic Structures in Half-Heusler Thermoelectric Materials. Research, 2020, 2020, 6375171.	5.7	32

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37	Visual Characterization of Anti-Reflective Coating on Solar Module Glass. , 2020, , .		2
38	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
39	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.8	236
40	Robocrystallographer: automated crystal structure text descriptions and analysis. MRS Communications, 2019, 9, 874-881.	1.8	30
41	Revelation of Inherently High Mobility Enables Mg₃Sb₂ as a Sustainable Alternative to nâ€Bi₂Te₃ Thermoelectrics. Advanced Science, 2019, 6, 1802286.	11.2	71
42	Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 2019, 571, 95-98.	27.8	590
43	Origins of ultralow thermal conductivity in 1-2-1-4 quaternary selenides. Journal of Materials Chemistry A, 2019, 7, 2589-2596.	10.3	28
44	Automatic Detection of Clear-Sky Periods From Irradiance Data. IEEE Journal of Photovoltaics, 2019, 9, 998-1005.	2.5	3
45	New horizons in thermoelectric materials: Correlated electrons, organic transport, machine learning, and more. Journal of Applied Physics, 2019, 125, .	2.5	50
46	Enhanced Thermochemical Heat Capacity of Liquids: Molecular to Macroscale Modeling. Nanoscale and Microscale Thermophysical Engineering, 2019, 23, 235-246.	2.6	4
47	Rocketsled: a software library for optimizing high-throughput computational searches. JPhys Materials, 2019, 2, 034002.	4.2	16
48	Geographic Assessment of Photovoltaic Module Environmental Degradation Stressors. , 2019, , .		2
49	Photovoltaic Degradation Climate Zones. , 2019, , .		11
50	A transferable machine-learning framework linking interstice distribution and plastic heterogeneity in metallic glasses. Nature Communications, 2019, 10, 5537.	12.8	56
51	Predicting the volumes of crystals. Computational Materials Science, 2018, 146, 184-192.	3.0	4
52	Low-Symmetry Rhombohedral GeTe Thermoelectrics. Joule, 2018, 2, 976-987.	24.0	402
53	First-principles calculations and experimental studies of XYZ₂ thermoelectric compounds: detailed analysis of van der Waals interactions. Journal of Materials Chemistry A, 2018, 6, 19502-19519.	10.3	20
54	Automatic Detection of Clear-sky Periods Using Ground and Satellite Based Solar Resource Data. , 2018, , .		6

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55	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
56	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
57	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
58	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
59	A computational assessment of the electronic, thermoelectric, and defect properties of bournonite (CuPbSbS₃) and related substitutions. Physical Chemistry Chemical Physics, 2017, 19, 6743-6756.	2.8	47
60	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. Npj Computational Materials, 2017, 3, .	8.7	145
61	Promising thermoelectric performance in van der Waals layered SnSe2. Materials Today Physics, 2017, 3, 127-136.	6.0	95
62	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	3.1	26
63	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
64	Metal phosphides as potential thermoelectric materials. Journal of Materials Chemistry C, 2017, 5, 12441-12456.	5.5	53
65	An ab initio electronic transport database for inorganic materials. Scientific Data, 2017, 4, 170085.	5.3	146
66	Assessing Local Structure Motifs Using Order Parameters for Motif Recognition, Interstitial Identification, and Diffusion Path Characterization. Frontiers in Materials, 2017, 4, .	2.4	54
67	Research Update: The materials genome initiative: Data sharing and the impact of collaborative ab initio databases. APL Materials, 2016, 4, .	5.1	115
68	Understanding thermoelectric properties from high-throughput calculations: trends, insights, and comparisons with experiment. Journal of Materials Chemistry C, 2016, 4, 4414-4426.	5.5	193
69	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. Energy and Environmental Science, 2016, 9, 3201-3209.	30.8	121
70	Computational predictions of energy materials using density functional theory. Nature Reviews Materials, 2016, 1, .	48.7	536
71	A Statistical Learning Framework for Materials Science: Application to Elastic Moduli of k-nary Inorganic Polycrystalline Compounds. Scientific Reports, 2016, 6, 34256.	3.3	178
72	The thermodynamic scale of inorganic crystalline metastability. Science Advances, 2016, 2, e1600225.	10.3	565

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73	New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships. Journal of Materials Research, 2016, 31, 977-994.	2.6	180
74	Large scale computational screening and experimental discovery of novel materials for high temperature CO₂ capture. Energy and Environmental Science, 2016, 9, 1346-1360.	30.8	61
75	YCuTe₂: a member of a new class of thermoelectric materials with CuTe₄-based layered structure. Journal of Materials Chemistry A, 2016, 4, 2461-2472.	10.3	52
76	A Community Contribution Framework for Sharing Materials Data with Materials Project. , 2015, , .		10
77	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
78	FireWorks: a dynamic workflow system designed for highâ€throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
79	First-principles study of electronic structure and photocatalytic properties of MnNiO₃ as an alkaline oxygen-evolution photocatalyst. Chemical Communications, 2015, 51, 2867-2870.	4.1	13
80	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
81	Relating voltage and thermal safety in Li-ion battery cathodes: a high-throughput computational study. Physical Chemistry Chemical Physics, 2015, 17, 5942-5953.	2.8	44
82	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
83	Supramolecular Perylene Bisimide-Polysulfide Gel Networks as Nanostructured Redox Mediators in Dissolved Polysulfide Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2015, 27, 6765-6770.	6.7	78
84	Computational and experimental investigation of TmAgTe₂and XYZ₂compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening. Journal of Materials Chemistry C, 2015, 3, 10554-10565.	5.5	99
85	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. Chemistry of Materials, 2015, 27, 6016-6021.	6.7	445
86	Spinel compounds as multivalent battery cathodes: a systematic evaluation based on ab initio calculations. Energy and Environmental Science, 2015, 8, 964-974.	30.8	430
87	The Materials Application Programming Interface (API): A simple, flexible and efficient API for materials data based on REpresentational State Transfer (REST) principles. Computational Materials Science, 2015, 97, 209-215.	3.0	322
88	New Lightâ€Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	19.5	124
89	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. Computational Materials Science, 2013, 68, 314-319.	3.0	2,392
90	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 2013, 1, .	5.1	6,913

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91	Performance of genetic algorithms in search for water splitting perovskites. Journal of Materials Science, 2013, 48, 6519-6534.	3.7	42
92	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. Chemistry of Materials, 2013, 25, 2064-2074.	6.7	72
93	Improved Capacity Retention for LiVO2by Cr Substitution. Journal of the Electrochemical Society, 2013, 160, A279-A284.	2.9	23
94	Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project. , 2012, , .		8
95	A Computational Investigation of Li₉M₃(P₂O₇)₃(PO₄)₂ (M) Tj ETQq1 1 0.7		64
96	Accuracy of density functional theory in predicting formation energies of ternary oxides from binary oxides and its implication on phase stability. Physical Review B, 2012, 85, .	3.2	380
97	From the computer to the laboratory: materials discovery and design using first-principles calculations. Journal of Materials Science, 2012, 47, 7317-7340.	3.7	154
98	Carbonophosphates: A New Family of Cathode Materials for Li-Ion Batteries Identified Computationally. Chemistry of Materials, 2012, 24, 2009-2016.	6.7	131
99	Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations. Journal of Materials Chemistry, 2011, 21, 17147.	6.7	204
100	Synthesis and Electrochemical Properties of Monoclinic LiMnBO[sub 3] as a Li Intercalation Material. Journal of the Electrochemical Society, 2011, 158, A309.	2.9	94
101	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
102	Evaluation of Tavorite-Structured Cathode Materials for Lithium-Ion Batteries Using High-Throughput Computing. Chemistry of Materials, 2011, 23, 3854-3862.	6.7	244
103	Formation enthalpies by mixing GGA and GGA+<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>U</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2011, 84, .	3.2	853
104	Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput ab Initio Calculations. Chemistry of Materials, 2011, 23, 3495-3508.	6.7	363
105	Data Mined Ionic Substitutions for the Discovery of New Compounds. Inorganic Chemistry, 2011, 50, 656-663.	4.0	300
106	Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials. Energy and Environmental Science, 2011, 4, 3680.	30.8	1,236
107	Finding Natureâ€™s Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory. Chemistry of Materials, 2010, 22, 3762-3767.	6.7	479
108	Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations. Electrochemistry Communications, 2010, 12, 427-430.	4.7	224

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109	Ab initio screening of metal sorbents for elemental mercury capture in syngas streams. Chemical Engineering Science, 2010, 65, 3025-3033.	3.8	48
110	Are you centered? An automatic crystal-centering method for high-throughput macromolecular crystallography. Journal of Synchrotron Radiation, 2007, 14, 355-360.	2.4	14