Anubhav Jain

List of Publications by Year
in descending order

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	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 2013, 1, .	5.1	6,913
2	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. Computational Materials Science, 2013, 68, 314-319.	3.0	2,392
3	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
4	Formation enthalpies by mixing GGA and GGA$+U$ calculations. Physical Review B, 2011, 84, .	3.2	853
5	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
6	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
7	Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 2019, 571, 95-98.	27.8	590
8	The thermodynamic scale of inorganic crystalline metastability. Science Advances, 2016, 2, e1600225.	10.3	565
9	Computational predictions of energy materials using density functional theory. Nature Reviews Materials, 2016, 1, .	48.7	536
10	Finding Nature's Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory. Chemistry of Materials, 2010, 22, 3762-3767.	6.7	479
11	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
12	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. Chemistry of Materials, 2015, 27, 6016-6021.	6.7	445
13	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
14	Low-Symmetry Rhombohedral GeTe Thermoelectrics. Joule, 2018, 2, 976-987.	24.0	402
15	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
16	FireWorks: a dynamic workflow system designed for high‐throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
17	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
18	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

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19	Data Mined Ionic Substitutions for the Discovery of New Compounds. Inorganic Chemistry, 2011, 50, 656-663.	4.0	300
20	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
21	Evaluation of Tavorite-Structured Cathode Materials for Lithium-Ion Batteries Using High-Throughput Computing. Chemistry of Materials, 2011, 23, 3854-3862.	6.7	244
22	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	13.6	240
23	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.8	236
24	Thermal stabilities of delithiated olivine MPO_4 (M=Fe, Mn) cathodes investigated using first principles calculations. Electrochemistry Communications, 2010, 12, 427-430.	4.7	224
25	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
26	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	8.7	207
27	Efficient calculation of carrier scattering rates from first principles. Nature Communications, 2021, 12, 2222.	12.8	205
28	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
29	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
30	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
31	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
32	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
33	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
34	An ab initio electronic transport database for inorganic materials. Scientific Data, 2017, 4, 170085.	5.3	146
35	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. Npj Computational Materials, 2017, 3, .	8.7	145
36	Carbonophosphates: A New Family of Cathode Materials for Li-Ion Batteries Identified Computationally. Chemistry of Materials, 2012, 24, 2009-2016.	6.7	131

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37	New Light‐Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	19.5	124
38	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. Energy and Environmental Science, 2016, 9, 3201-3209.	30.8	121
39	A critical examination of compound stability predictions from machine-learned formation energies. Npj Computational Materials, 2020, 6, .	8.7	119
40	Research Update: The materials genome initiative: Data sharing and the impact of collaborative *ab initio* databases. APL Materials, 2016, 4, .	5.1	115
41	Computational and experimental investigation of $TmAgTe_2$ and XYZ_2 compounds, 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
42	Benchmarking materials property prediction methods: the Matbench test set and Automatminer reference algorithm. Npj Computational Materials, 2020, 6, .	8.7	96
43	Promising thermoelectric performance in van der Waals layered SnSe2. Materials Today Physics, 2017, 3, 127-136.	6.0	95
44	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
45	Supramolecular Perylene Bisimide-Polysulfide Gel Networks as Nanostructured Redox Mediators in Dissolved Polysulfide Lithium‒Sulfur Batteries. Chemistry of Materials, 2015, 27, 6765-6770.	6.7	78
46	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. Chemistry of Materials, 2013, 25, 2064-2074.	6.7	72
47	Revelation of Inherently High Mobility Enables Mg_3Sb_2 as a Sustainable Alternative to n‐Bi_2Te_3 Thermoelectrics. Advanced Science, 2019, 6, 1802286.	11.2	71
48	A Computational Investigation of $Li_9M_3(P_2O_7)_3(PO_4)_2$ (M Tj ETQq0 0 0 rgBT		
49	Large scale computational screening and experimental discovery of novel materials for high temperature CO_2 capture. Energy and Environmental Science, 2016, 9, 1346-1360.	30.8	61
50	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
51	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
52	A transferable machine-learning framework linking interstice distribution and plastic heterogeneity in metallic glasses. Nature Communications, 2019, 10, 5537.	12.8	56
53	Assessing Local Structure Motifs Using Order Parameters for Motif Recognition, Interstitial Identification, and Diffusion Path Characterization. Frontiers in Materials, 2017, 4, .	2.4	54
54	Metal phosphides as potential thermoelectric materials. Journal of Materials Chemistry C, 2017, 5, 12441-12456.	5.5	53

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55	YCuTe$_2$: a member of a new class of thermoelectric materials with CuTe$_4$-based layered structure. Journal of Materials Chemistry A, 2016, 4, 2461-2472.	10.3	52
56	When band convergence is not beneficial for thermoelectrics. Nature Communications, 2021, 12, 3425.	12.8	51
57	A framework for quantifying uncertainty in DFT energy corrections. Scientific Reports, 2021, 11, 15496.	3.3	51
58	New horizons in thermoelectric materials: Correlated electrons, organic transport, machine learning, and more. Journal of Applied Physics, 2019, 125, .	2.5	50
59	Ab initio screening of metal sorbents for elemental mercury capture in syngas streams. Chemical Engineering Science, 2010, 65, 3025-3033.	3.8	48
60	A computational assessment of the electronic, thermoelectric, and defect properties of bournonite (CuPbSbS$_3$) and related substitutions. Physical Chemistry Chemical Physics, 2017, 19, 6743-6756.	2.8	47
61	Toward a Mechanistic Model of Solid–Electrolyte Interphase Formation and Evolution in Lithium-Ion Batteries. ACS Energy Letters, 2022, 7, 1446-1453.	17.4	46
62	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science. Patterns, 2022, 3, 100488.	5.9	46
63	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
64	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
65	Performance of genetic algorithms in search for water splitting perovskites. Journal of Materials Science, 2013, 48, 6519-6534.	3.7	42
66	Compromise between band structure and phonon scattering in efficient n-Mg3Sb2-Bi thermoelectrics. Materials Today Physics, 2021, 18, 100362.	6.0	41
67	An automatically curated first-principles database of ferroelectrics. Scientific Data, 2020, 7, 72.	5.3	39
68	Experimental validation of high thermoelectric performance in RECuZnP2 predicted by high-throughput DFT calculations. Materials Horizons, 2021, 8, 209-215.	12.2	38
69	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
70	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
71	Machine Learning Chemical Guidelines for Engineering Electronic Structures in Half-Heusler Thermoelectric Materials. Research, 2020, 2020, 6375171.	5.7	32
72	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31

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73	Robocrystallographer: automated crystal structure text descriptions and analysis. MRS Communications, 2019, 9, 874-881.	1.8	30
74	Computational discovery of promising new n-type dopable ABX Zintl thermoelectric materials. Materials Horizons, 2020, 7, 1809-1818.	12.2	30
75	Origins of ultralow thermal conductivity in 1-2-1-4 quaternary selenides. Journal of Materials Chemistry A, 2019, 7, 2589-2596.	10.3	28
76	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	3.1	26
77	IFermi: A python library for Fermi surface generation and analysis. Journal of Open Source Software, 2021, 6, 3089.	4.6	26
78	High Thermoelectric Performance and Defect Energetics of Multipocketed Full Heusler Compounds. Physical Review Applied, 2020, 14, .	3.8	25
79	Optimal band structure for thermoelectrics with realistic scattering and bands. Npj Computational Materials, 2021, 7, .	8.7	25
80	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
81	Text-mined dataset of gold nanoparticle synthesis procedures, morphologies, and size entities. Scientific Data, 2022, 9, .	5.3	24
82	Improved Capacity Retention for LiVO2 by Cr Substitution. Journal of the Electrochemical Society, 2013, 160, A279-A284.	2.9	23
83	Reducing Interanalyst Variability in Photovoltaic Degradation Rate Assessments. IEEE Journal of Photovoltaics, 2020, 10, 206-212.	2.5	22
84	First-principles calculations and experimental studies of XYZ_2 thermoelectric compounds: detailed analysis of van der Waals interactions. Journal of Materials Chemistry A, 2018, 6, 19502-19519.	10.3	20
85	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
86	Gapped metals as thermoelectric materials revealed by high-throughput screening. Journal of Materials Chemistry A, 2020, 8, 17579-17594.	10.3	19
87	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
88	Automated defect identification in electroluminescence images of solar modules. Solar Energy, 2022, 242, 20-29.	6.1	18
89	Rocketsled: a software library for optimizing high-throughput computational searches. JPhys Materials, 2019, 2, 034002.	4.2	16
90	Are you centered? An automatic crystal-centering method for high-throughput macromolecular crystallography. Journal of Synchrotron Radiation, 2007, 14, 355-360.	2.4	14

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91	Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of $Na_3V_2(PO_4)_2F_3$. Chemistry of Materials, 2020, 32, 8981-8992.	6.7	14
92	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
93	First-principles study of electronic structure and photocatalytic properties of $MnNiO_3$ as an alkaline oxygen-evolution photocatalyst. Chemical Communications, 2015, 51, 2867-2870.	4.1	13
94	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
95	Photovoltaic Degradation Climate Zones. , 2019, , .		11
96	A Community Contribution Framework for Sharing Materials Data with Materials Project. , 2015, , .		10
97	Phase-Transition-Enhanced Thermoelectric Transport in Rickardite Mineral $Cu_{3-x}Te_2$. Chemistry of Materials, 2021, 33, 1832-1841.	6.7	9
98	Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project. , 2012, , .		8
99	Nondestructive Characterization of Antireflective Coatings on PV Modules. IEEE Journal of Photovoltaics, 2021, 11, 760-769.	2.5	7
100	Automatic Detection of Clear-sky Periods Using Ground and Satellite Based Solar Resource Data. , 2018, , .		6
101	A simple model for the entropy of melting of monatomic liquids. Applied Physics Letters, 2021, 118, .	3.3	6
102	Photovoltaic String Sizing Using Site-Specific Modeling. IEEE Journal of Photovoltaics, 2020, 10, 888-897.	2.5	5
103	Predicting the volumes of crystals. Computational Materials Science, 2018, 146, 184-192.	3.0	4
104	Enhanced Thermochemical Heat Capacity of Liquids: Molecular to Macroscale Modeling. Nanoscale and Microscale Thermophysical Engineering, 2019, 23, 235-246.	2.6	4
105	Aqueous Diels–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
106	Automatic Detection of Clear-Sky Periods From Irradiance Data. IEEE Journal of Photovoltaics, 2019, 9, 998-1005.	2.5	3
107	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
108	Geographic Assessment of Photovoltaic Module Environmental Degradation Stressors. , 2019, , .		2

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109	Visual Characterization of Anti-Reflective Coating on Solar Module Glass. , 2020, , .		2
110	Thermal fluids with high specific heat capacity through reversible Diels-Alder reactions. IScience, 2022, 25, 103540.	4.1	2