Kristin A Persson

List of Publications by Year
in descending order

		8181	3915
213	33,347	76	177
papers	citations	h-index	g-index

220	220	220	26949
all docs	docs citations	times ranked	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	Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. Chemical Reviews, 2017, 117, 4287-4341.	47.7	914
4	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
5	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
6	Promises and Challenges of Next-Generation â€œBeyond Li-ionâ€•Batteries for Electric Vehicles and Grid Decarbonization. Chemical Reviews, 2021, 121, 1623-1669.	47.7	769
7	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
8	Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 2019, 571, 95-98.	27.8	590
9	Surface energies of elemental crystals. Scientific Data, 2016, 3, 160080.	5.3	583
10	The thermodynamic scale of inorganic crystalline metastability. Science Advances, 2016, 2, e1600225.	10.3	565
11	Computational predictions of energy materials using density functional theory. Nature Reviews Materials, 2016, 1, .	48.7	536
12	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
13	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
14	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. Chemistry of Materials, 2015, 27, 6016-6021.	6.7	445
15	The origin of high electrolyteâ€“electrode interfacial resistances in lithium cells containing garnet type solid electrolytes. Physical Chemistry Chemical Physics, 2014, 16, 18294-18300.	2.8	431
16	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
17	FireWorks: a dynamic workflow system designed for highâ€throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
18	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369

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19	Predicting Crystal Structures with Data Mining of Quantum Calculations. Physical Review Letters, 2003, 91, 135503.	7.8	354
20	A high capacity thiospinel cathode for Mg batteries. Energy and Environmental Science, 2016, 9, 2273-2277.	30.8	349
21	Effect of Surface Microstructure on Electrochemical Performance of Garnet Solid Electrolytes. ACS Applied Materials & Interfaces, 2015, 7, 2073-2081.	8.0	347
22	Prediction of solid-aqueous equilibria: Scheme to combine first-principles calculations of solids with experimental aqueous states. Physical Review B, 2012, 85, .	3.2	342
23	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
24	Uncharted Waters: Super-Concentrated Electrolytes. Joule, 2020, 4, 69-100.	24.0	305
25	Combining theory and experiment in lithiumâ€“sulfur batteries: Current progress and future perspectives. Materials Today, 2019, 22, 142-158.	14.2	301
26	First principles high throughput screening of oxynitrides for water-splitting photocatalysts. Energy and Environmental Science, 2013, 6, 157-168.	30.8	290
27	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
28	The Coupling between Stability and Ion Pair Formation in Magnesium Electrolytes from First-Principles Quantum Mechanics and Classical Molecular Dynamics. Journal of the American Chemical Society, 2015, 137, 3411-3420.	13.7	259
29	A Review on Challenges and Successes in Atomic-Scale Design of Catalysts for Electrochemical Synthesis of Hydrogen Peroxide. ACS Catalysis, 2020, 10, 7495-7511.	11.2	254
30	Wide Band Gap Chalcogenide Semiconductors. Chemical Reviews, 2020, 120, 4007-4055.	47.7	246
31	The influence of FEC on the solvation structure and reduction reaction of LiPF6/EC electrolytes and its implication for solid electrolyte interphase formation. Nano Energy, 2019, 64, 103881.	16.0	239
32	Mechanistic insights into chemical and photochemical transformations of bismuth vanadate photoanodes. Nature Communications, 2016, 7, 12012.	12.8	231
33	Machine Learning for Materials Scientists: An Introductory Guide toward Best Practices. Chemistry of Materials, 2020, 32, 4954-4965.	6.7	224
34	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
35	Interrelationships among Grain Size, Surface Composition, Air Stability, and Interfacial Resistance of Al-Substituted Li₇La₃Zr₂O₁₂ Solid Electrolytes. ACS Applied Materials & Interfaces, 2015, 7, 17649-17655.	8.0	220
36	Energy storage emerging: A perspective from the Joint Center for Energy Storage Research. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 12550-12557.	7.1	218

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37	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
38	Efficient calculation of carrier scattering rates from first principles. Nature Communications, 2021, 12, 2222.	12.8	205
39	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	5.3	201
40	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
41	Materials science with large-scale data and informatics: Unlocking new opportunities. MRS Bulletin, 2016, 41, 399-409.	3.5	192
42	A database to enable discovery and design of piezoelectric materials. Scientific Data, 2015, 2, 150053.	5.3	191
43	Nucleation of metastable aragonite CaCO ₃ in seawater. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3199-3204.	7.1	187
44	Origin of Electrochemical, Structural, and Transport Properties in Nonaqueous Zinc Electrolytes. ACS Applied Materials & Interfaces, 2016, 8, 3021-3031.	8.0	181
45	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
46	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
47	Structural and Chemical Evolution of the Layered Liâ€Excess Li_xMnO₃ as a Function of Li Content from Firstâ€Principles Calculations. Advanced Energy Materials, 2014, 4, 1400498.	19.5	173
48	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
49	Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3040-3043.	7.1	157
50	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
51	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. Npj Computational Materials, 2017, 3, .	8.7	145
52	High-throughput screening of inorganic compounds for the discovery of novel dielectric and optical materials. Scientific Data, 2017, 4, 160134.	5.3	140
53	Named Entity Recognition and Normalization Applied to Large-Scale Information Extraction from the Materials Science Literature. Journal of Chemical Information and Modeling, 2019, 59, 3692-3702.	5.4	136
54	Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries. Energy and Environmental Science, 2015, 8, 3718-3730.	30.8	131

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55	Ion Transport and the True Transference Number in Nonaqueous Polyelectrolyte Solutions for Lithium Ion Batteries. ACS Central Science, 2019, 5, 1250-1260.	11.3	126
56	Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery. Nature Communications, 2019, 10, 443.	12.8	125
57	Solvation structure and energetics of electrolytes for multivalent energy storage. Physical Chemistry Chemical Physics, 2014, 16, 21941-21945.	2.8	124
58	High-throughput density-functional perturbation theory phonons for inorganic materials. Scientific Data, 2018, 5, 180065.	5.3	122
59	Materials design of perovskite solid solutions for thermochemical applications. Energy and Environmental Science, 2019, 12, 1369-1384.	30.8	122
60	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
61	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. Energy and Environmental Science, 2016, 9, 3201-3209.	30.8	121
62	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. Chemistry of Materials, 2017, 29, 3375-3379.	6.7	117
63	Research Update: The materials genome initiative: Data sharing and the impact of collaborative ab initio databases. APL Materials, 2016, 4, .	5.1	115
64	Grain boundary properties of elemental metals. Acta Materialia, 2020, 186, 40-49.	7.9	115
65	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
66	Computational prediction of new auxetic materials. Nature Communications, 2017, 8, 323.	12.8	105
67	High-throughput Computational Study of Halide Double Perovskite Inorganic Compounds. Chemistry of Materials, 2019, 31, 5392-5401.	6.7	102
68	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
69	Unraveling the Nanoscale Heterogeneity of Solid Electrolyte Interphase Using Tip-Enhanced Raman Spectroscopy. Joule, 2019, 3, 2001-2019.	24.0	99
70	Rutile Alloys in the Mnâ€“Sbâ€“O System Stabilize Mn³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	11.2	97
71	Distinct Solidâ€Electrolyteâ€Interphases on Sn (100) and (001) Electrodes Studied by Soft Xâ€Ray Spectroscopy. Advanced Materials Interfaces, 2014, 1, 1300115.	3.7	94
72	High-throughput computational X-ray absorption spectroscopy. Scientific Data, 2018, 5, 180151.	5.3	94

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73	Predicting defect behavior in B2 intermetallics by merging ab initio modeling and machine learning. Npj Computational Materials, 2016, 2, .	8.7	90
74	â€œRocking-Chairâ€•Type Metal Hybrid Supercapacitors. ACS Applied Materials & Interfaces, 2016, 8, 30853-30862.	8.0	86
75	Anisotropic work function of elemental crystals. Surface Science, 2019, 687, 48-55.	1.9	84
76	Automated generation and ensemble-learned matching of X-ray absorption spectra. Npj Computational Materials, 2018, 4, .	8.7	82
77	Garnet Electrolyte Surface Degradation and Recovery. ACS Applied Energy Materials, 2018, 1, 7244-7252.	5.1	81
78	Enhanced Stability of the Carba-closo-dodecaborate Anion for High-Voltage Battery Electrolytes through Rational Design. Journal of the American Chemical Society, 2018, 140, 11076-11084.	13.7	80
79	Computational Approach for Epitaxial Polymorph Stabilization through Substrate Selection. ACS Applied Materials & Interfaces, 2016, 8, 13086-13093.	8.0	78
80	The existence and impact of persistent ferroelectric domains in MAPbI ₃. Science Advances, 2019, 5, eaas9311.	10.3	77
81	Ab initiostudy of the composition dependence of the pressure-induced spin transition in the (Mg1â^'x,Fex)O system. Geophysical Research Letters, 2006, 33, .	4.0	76
82	Beyond Local Solvation Structure: Nanometric Aggregates in Battery Electrolytes and Their Effect on Electrolyte Properties. ACS Energy Letters, 2022, 7, 461-470.	17.4	75
83	Transport in Superconcentrated LiPF₆ and LiBF₄/Propylene Carbonate Electrolytes. ACS Energy Letters, 2019, 4, 2843-2849.	17.4	71
84	Additiveâ€Free, Lowâ€Temperature Crystallization of Stable Î±â€FAPbI₃ Perovskite. Advanced Materials, 2022, 34, e2107850.	21.0	71
85	A high-throughput framework for determining adsorption energies on solid surfaces. Npj Computational Materials, 2017, 3, .	8.7	70
86	High-throughput prediction of the ground-state collinear magnetic order of inorganic materials using Density Functional Theory. Npj Computational Materials, 2019, 5, .	8.7	69
87	Efficient Pourbaix diagrams of many-element compounds. Physical Chemistry Chemical Physics, 2019, 21, 25323-25327.	2.8	69
88	Revealing the coupled cation interactions behind the electrochemical profile of LixNi0.5Mn1.5O4. Energy and Environmental Science, 2012, 5, 6047.	30.8	67
89	The lithiation process and Li diffusion in amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:r and Si from first-principles. Electrochimica Acta, 2020, 331, 135344.	5.2	66
90	Concentration dependent electrochemical properties and structural analysis of a simple magnesium electrolyte: magnesium bis(trifluoromethane sulfonyl)imide in diglyme. RSC Advances, 2016, 6, 113663-113670.	3.6	65

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91	Conformational Entropy as a Means to Control the Behavior of Poly(diketoenamine) Vitrimers In and Out of Equilibrium. Angewandte Chemie - International Edition, 2020, 59, 735-739.	13.8	64
92	Tuning the Solvation Structure in Aqueous Zinc Batteries to Maximize Zn-Ion Intercalation and Optimize Dendrite-Free Zinc Plating. ACS Energy Letters, 2022, 7, 533-540.	17.4	62
93	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	19.5	61
94	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
95	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€"A Review. Topics in Current Chemistry, 2018, 376, 19.	5.8	61
96	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
97	Widening Electrochemical Window of Mg Salt by Weakly Coordinating Perfluoroalkoxyaluminate Anion for Mg Battery Electrolyte. Journal of the Electrochemical Society, 2019, 166, A1510-A1519.	2.9	60
98	Anomalous metal segregation in lithium-rich material provides design rules for stable cathode in lithium-ion battery. Nature Communications, 2019, 10, 1650.	12.8	60
99	Revealing the Intrinsic Li Mobility in the Li₂MnO₃ Lithium-Excess Material. Chemistry of Materials, 2016, 28, 2081-2088.	6.7	59
100	Solid-Solution Li Intercalation as a Function of Cation Order/Disorder in the High-Voltage LixNi0.5Mn1.5O4 Spinel. Chemistry of Materials, 2013, 25, 2885-2889.	6.7	56
101	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. Physical Chemistry Chemical Physics, 2016, 18, 9349-9352.	2.8	56
102	Alleviating oxygen evolution from Li-excess oxide materials through theory-guided surface protection. Nature Communications, 2018, 9, 4597.	12.8	56
103	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. Chemistry of Materials, 2019, 31, 2308-2319.	6.7	54
104	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
105	A framework for quantifying uncertainty in DFT energy corrections. Scientific Reports, 2021, 11, 15496.	3.3	51
106	Oxidation Protection with Amorphous Surface Oxides: Thermodynamic Insights from Ab Initio Simulations on Aluminum. ACS Applied Materials & Interfaces, 2018, 10, 3039-3045.	8.0	50
107	Incorporating Electronic Information into Machine Learning Potential Energy Surfaces via Approaching the Ground-State Electronic Energy as a Function of Atom-Based Electronic Populations. Journal of Chemical Theory and Computation, 2020, 16, 4256-4270.	5.3	50
108	Ion Correlations and Their Impact on Transport in Polymer-Based Electrolytes. Macromolecules, 2021, 54, 2575-2591.	4.8	50

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109	Intrinsic chemical reactivity of solid-electrolyte interphase components in siliconâ€“lithium alloy anode batteries probed by FTIR spectroscopy. Journal of Materials Chemistry A, 2020, 8, 7897-7906.	10.3	49
110	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49
111	Benchmarking density functional perturbation theory to enable high-throughput screening of materials for dielectric constant and refractive index. Physical Review B, 2016, 93, .	3.2	46
112	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
113	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science. Patterns, 2022, 3, 100488.	5.9	46
114	Materials Genomics Screens for Adaptive Ion Transport Behavior by Redox-Switchable Microporous Polymer Membranes in Lithiumâ€“Sulfur Batteries. ACS Central Science, 2017, 3, 399-406.	11.3	44
115	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. ACS Energy Letters, 2020, 5, 200-206.	17.4	44
116	Enhancing surface oxygen retention through theory-guided doping selection in Li_{1â^'x}NiO₂ for next-generation lithium-ion batteries. Journal of Materials Chemistry A, 2020, 8, 23293-23303.	10.3	44
117	A graph-based network for predicting chemical reaction pathways in solid-state materials synthesis. Nature Communications, 2021, 12, 3097.	12.8	44
118	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
119	The Interplay between Salt Association and the Dielectric Properties of Low Permittivity Electrolytes: The Case of LiPF₆ and LiAsF₆ in Dimethyl Carbonate. Journal of Physical Chemistry C, 2018, 122, 1990-1994.	3.1	43
120	High-throughput predictions of metalâ€“organic framework electronic properties: theoretical challenges, graph neural networks, and data exploration. Npj Computational Materials, 2022, 8, .	8.7	43
121	Onsager Transport Coefficients and Transference Numbers in Polyelectrolyte Solutions and Polymerized Ionic Liquids. Macromolecules, 2020, 53, 9503-9512.	4.8	42
122	Surface Morphology and Surface Stability against Oxygen Loss of the Lithium-Excess Li₂MnO₃ Cathode Material as a Function of Lithium Concentration. ACS Applied Materials & Interfaces, 2016, 8, 25595-25602.	8.0	38
123	25Mg NMR and computational modeling studies of the solvation structures and molecular dynamics in magnesium based liquid electrolytes. Nano Energy, 2018, 46, 436-446.	16.0	37
124	The critical role of configurational flexibility in facilitating reversible reactive metal deposition from borohydride solutions. Journal of Materials Chemistry A, 2020, 8, 7235-7244.	10.3	37
125	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. ACS Energy Letters, 2017, 2, 2307-2312.	17.4	36
126	Elucidating Non-aqueous Solvent Stability and Associated Decomposition Mechanisms for Mg Energy Storage Applications From First-Principles. Frontiers in Chemistry, 2019, 7, 175.	3.6	36

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127	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
128	Effects of Anion Mobility on Electrochemical Behaviors of Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
129	High-throughput search for magnetic and topological order in transition metal oxides. Science Advances, 2020, 6, .	10.3	35
130	Transport Phenomena in Low Temperature Lithium-Ion Battery Electrolytes. Journal of the Electrochemical Society, 2021, 168, 080501.	2.9	35
131	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
132	An improved symmetry-based approach to reciprocal space path selection in band structure calculations. Npj Computational Materials, 2020, 6, .	8.7	33
133	Ionic Conduction Mechanism and Design of Metalâ€“Organic Framework Based Quasi-Solid-State Electrolytes. Journal of the American Chemical Society, 2022, 144, 13446-13450.	13.7	33
134	Evaluation of thermodynamic equations of state across chemistry and structure in the materials project. Npj Computational Materials, 2018, 4, .	8.7	32
135	Exploring the Pb_{1â^'}_xSr_xHfO₃ System and Potential for High Capacitive Energy Storage Density and Efficiency. Advanced Materials, 2022, 34, e2105967.	21.0	32
136	Investigation of Solvent Type and Salt Addition in High Transference Number Nonaqueous Polyelectrolyte Solutions for Lithium Ion Batteries. Macromolecules, 2018, 51, 8761-8771.	4.8	31
137	Alkyltin clusters: the less symmetric Keggin isomers. Dalton Transactions, 2018, 47, 9804-9813.	3.3	31
138	An Electrifying Choice for the 2019 Chemistry Nobel Prize: Goodenough, Whittingham, and Yoshino. Chemistry of Materials, 2019, 31, 8577-8581.	6.7	31
139	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31
140	Performance comparison of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>r</mml:mi></mml:mrow><mml:mn>2</mml and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow. Physical Review Materials, 2022, 6, .	2.4	31
141	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	17.4	30
142	The solvation structure, transport properties and reduction behavior of carbonate-based electrolytes of lithium-ion batteries. Chemical Science, 2021, 12, 14740-14751.	7.4	29
143	Data-Driven Prediction of Formation Mechanisms of Lithium Ethylene Monocarbonate with an Automated Reaction Network. Journal of the American Chemical Society, 2021, 143, 13245-13258.	13.7	29
144	Understanding the Role of SEI Layer in Low-Temperature Performance of Lithium-Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 11910-11918.	8.0	29

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145	Ion Pairing and Redissociaton in Low-Permittivity Electrolytes for Multivalent Battery Applications. Journal of Physical Chemistry Letters, 2020, 11, 2046-2052.	4.6	28
146	Group additivity-Pourbaix diagrams advocate thermodynamically stable nanoscale clusters in aqueous environments. Nature Communications, 2017, 8, 15852.	12.8	27
147	Dynamic Control of Optical Response in Layered Metal Chalcogenide Nanoplates. Nano Letters, 2016, 16, 488-496.	9.1	26
148	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	3.1	26
149	Combinatorial Tuning of Structural and Optoelectronic Properties in Cu Zn1â^'S. Matter, 2019, 1, 862-880.	10.0	26
150	Evaluation of Amorphous Oxide Coatings for High-Voltage Li-Ion Battery Applications Using a First-Principles Framework. ACS Applied Materials & Interfaces, 2020, 12, 35748-35756.	8.0	26
151	Selectivity in Yttrium Manganese Oxide Synthesis via Local Chemical Potentials in Hyperdimensional Phase Space. Journal of the American Chemical Society, 2021, 143, 15185-15194.	13.7	25
152	Promises and perils of computational materials databases. Nature Computational Science, 2021, 1, 3-5.	8.0	25
153	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24
154	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
155	In-situ resonant band engineering of solution-processed semiconductors generates high performance n-type thermoelectric nano-inks. Nature Communications, 2020, 11, 2069.	12.8	23
156	Toward Accurate Modeling of the Effect of Ion-Pair Formation on Solute Redox Potential. Journal of Chemical Theory and Computation, 2016, 12, 4501-4508.	5.3	22
157	Fast Mg2+ diffusion in Mo3(PO4)3O for Mg batteries. Chemical Communications, 2017, 53, 7998-8001.	4.1	22
158	Defect-Accommodating Intermediates Yield Selective Low-Temperature Synthesis of YMnO₃ Polymorphs. Inorganic Chemistry, 2020, 59, 13639-13650.	4.0	22
159	Strain-Mediated Interfacial Dynamics during Auâ€“PbS Coreâ€“Shell Nanostructure Formation. ACS Nano, 2016, 10, 6235-6240.	14.6	21
160	Mechanical Properties and Chemical Reactivity of Li_xSiO_y Thin Films. ACS Applied Materials & Interfaces, 2018, 10, 38558-38564.	8.0	21
161	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
162	ChemEnv: a fast and robust coordination environment identification tool. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 683-695.	1.1	21

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163	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
164	Two-dimensional forms of robust CO2 reduction photocatalysts. Npj 2D Materials and Applications, 2020, 4, .	7.9	20
165	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
166	PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds. Computer Physics Communications, 2015, 193, 118-123.	7.5	18
167	Preferential Solvation of an Asymmetric Redox Molecule. Journal of Physical Chemistry C, 2016, 120, 27834-27839.	3.1	18
168	A charge-density-based general cation insertion algorithm for generating new Li-ion cathode materials. Npj Computational Materials, 2020, 6, .	8.7	18
169	From Waste-Heat Recovery to Refrigeration: Compositional Tuning of Magnetocaloric Mn_{1+x}Sb. Chemistry of Materials, 2020, 32, 1243-1249.	6.7	18
170	Discovery and Characterization of a Pourbaix-Stable, 1.8 eV Direct Gap Bismuth Manganate Photoanode. Chemistry of Materials, 2017, 29, 10027-10036.	6.7	17
171	Quantifying Species Populations in Multivalent Borohydride Electrolytes. Journal of Physical Chemistry B, 2021, 125, 3644-3652.	2.6	17
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