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	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
2	Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining. Chemical Science, 2022, 13, 1446-1458.	7.4	17
3	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:mn> and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow. Physical Review Materials, 2022, 6, .	2.4	31
4	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
5	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 674-686.	2.8	13
6	Additiveâ€Free, Lowâ€Temperature Crystallization of Stable Î±â€FAPbI₃ Perovskite. Advanced Materials, 2022, 34, e2107850.	21.0	71
7	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
8	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
9	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science. Patterns, 2022, 3, 100488.	5.9	46
10	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
11	NGenE 2021: Electrochemistry Is Everywhere. ACS Energy Letters, 2022, 7, 368-374.	17.4	6
12	Role of disorder in the synthesis of metastable zinc zirconium nitrides. Physical Review Materials, 2022, 6, .	2.4	14
13	Reaction Selectivity in Cometathesis: Yttrium Manganese Oxides. Chemistry of Materials, 2022, 34, 4694-4702.	6.7	4
14	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
15	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
16	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
17	A chemically consistent graph architecture for massive reaction networks applied to solid-electrolyte interphase formation. Chemical Science, 2021, 12, 4931-4939.	7.4	36
18	Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures. Inorganic Chemistry, 2021, 60, 1590-1603.	4.0	31

#	Article	IF	Citations
19	Metastable Ta₂N₃ with highly tunable electrical conductivity via oxygen incorporation. Materials Horizons, 2021, 8, 1744-1755.	12.2	6
20	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
21	Ion Correlations and Their Impact on Transport in Polymer-Based Electrolytes. Macromolecules, 2021, 54, 2575-2591.	4.8	50
22	Evaluating Materials Design Parameters of Hole-Selective Contacts for Silicon Heterojunction Solar Cells. IEEE Journal of Photovoltaics, 2021, 11, 247-258.	2.5	7
23	Quantifying Species Populations in Multivalent Borohydride Electrolytes. Journal of Physical Chemistry B, 2021, 125, 3644-3652.	2.6	17
24	Efficient calculation of carrier scattering rates from first principles. Nature Communications, 2021, 12, 2222.	12.8	205
25	Lowering Ternary Oxide Synthesis Temperatures by Solid-State Cometathesis Reactions. Chemistry of Materials, 2021, 33, 3692-3701.	6.7	14
26	A graph-based network for predicting chemical reaction pathways in solid-state materials synthesis. Nature Communications, 2021, 12, 3097.	12.8	44
27	Prospects for Employing Lithium Copper Phosphates as High-Voltage Li-Ion Cathodes. Journal of Physical Chemistry C, 2021, 125, 13123-13130.	3.1	0
28	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
29	Advancing Electrolyte Solution Chemistry and Interfacial Electrochemistry of Divalent Metal Batteries. ChemElectroChem, 2021, 8, 3013-3029.	3.4	13
30	Automated Adsorption Workflow for Semiconductor Surfaces and the Application to Zinc Telluride. Journal of Chemical Information and Modeling, 2021, 61, 3908-3916.	5.4	11
31	Online Interactive Platform for COVID-19 Literature Visual Analytics: Platform Development Study. Journal of Medical Internet Research, 2021, 23, e26995.	4.3	2
32	A framework for quantifying uncertainty in DFT energy corrections. Scientific Reports, 2021, 11, 15496.	3.3	51
33	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
34	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	5.3	19
35	Effective Local Geometry Descriptor for 29Si NMR Q4 Anisotropy. Journal of Physical Chemistry C, 2021, 125, 19481-19488.	3.1	3
36	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49

#	Article	IF	Citations
37	Transport Phenomena in Low Temperature Lithium-Ion Battery Electrolytes. Journal of the Electrochemical Society, 2021, 168, 080501.	2.9	35
38	Role of Fluorine in Chemomechanics of Cation-Disordered Rocksalt Cathodes. Chemistry of Materials, 2021, 33, 7028-7038.	6.7	8
39	Silicon Anodes with Improved Calendar Life Enabled By Multivalent Additives. Advanced Energy Materials, 2021, 11, 2101820.	19.5	17
40	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
41	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. Chemistry of Materials, 2021, 33, 7242-7253.	6.7	7
42	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
43	Synthesis of model sodium sulfide films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, 053404.	2.1	3
44	BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules. Chemical Science, 2021, 12, 1858-1868.	7.4	44
45	Promises and perils of computational materials databases. Nature Computational Science, 2021, 1, 3-5.	8.0	25
46	Aqueous Stability of Zirconium Clusters, Including the Zr(IV) Hexanuclear Hydrolysis Complex [Zr₆O₄(OH)₄(H₂O)₂₄]¹²⁺, from Density Functional Theory. Inorganic Chemistry, 2021, 60, 15456-15466.	4.0	5
47	A Theoretical Model for Computing Freezing Point Depression of Lithium-Ion Battery Electrolytes. Journal of the Electrochemical Society, 2021, 168, 120532.	2.9	6
48	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
49	Grain boundary properties of elemental metals. Acta Materialia, 2020, 186, 40-49.	7.9	115
50	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. ACS Energy Letters, 2020, 5, 200-206.	17.4	44
51	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
52	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
53	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
54	Onsager Transport Coefficients and Transference Numbers in Polyelectrolyte Solutions and Polymerized Ionic Liquids. Macromolecules, 2020, 53, 9503-9512.	4.8	42

#	Article	IF	Citations
55	Li₅VF₄(SO₄)₂: A Prototype High-Voltage Li-Ion Cathode. ACS Applied Materials & Interfaces, 2020, 12, 48662-48668.	8.0	1
56	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
57	First-principles study of CaB₁₂H₁₂ as a potential solid-state conductor for Ca. Physical Chemistry Chemical Physics, 2020, 22, 27600-27604.	2.8	8
58	Two-dimensional forms of robust CO2 reduction photocatalysts. Npj 2D Materials and Applications, 2020, 4, .	7.9	20
59	An improved symmetry-based approach to reciprocal space path selection in band structure calculations. Npj Computational Materials, 2020, 6, .	8.7	33
60	A charge-density-based general cation insertion algorithm for generating new Li-ion cathode materials. Npj Computational Materials, 2020, 6, .	8.7	18
61	Defect-Accommodating Intermediates Yield Selective Low-Temperature Synthesis of YMnO₃ Polymorphs. Inorganic Chemistry, 2020, 59, 13639-13650.	4.0	22
62	High-throughput search for magnetic and topological order in transition metal oxides. Science Advances, 2020, 6, .	10.3	35
63	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
64	Machine Learning for Materials Scientists: An Introductory Guide toward Best Practices. Chemistry of Materials, 2020, 32, 4954-4965.	6.7	224
65	Sputtered p-Type Cu_xZn_{1â€“x}S Back Contact to CdTe Solar Cells. ACS Applied Energy Materials, 2020, 3, 5427-5438.	5.1	11
66	Enabling materials informatics for 29Si solid-state NMR of crystalline materials. Npj Computational Materials, 2020, 6, .	8.7	11
67	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
68	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
69	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
70	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
71	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
72	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	17.4	30

#	Article	IF	Citations
73	Origin of Disorder Tolerance in Piezoelectric Materials and Design of Polar Systems. Chemistry of Materials, 2020, 32, 2836-2842.	6.7	4
74	Combinatorial screening yields discovery of 29 metal oxide photoanodes for solar fuel generation. Journal of Materials Chemistry A, 2020, 8, 4239-4243.	10.3	13
75	Tunable valleytronics with symmetry-retaining high polarization degree in SnSxSe1â^'x model system. Applied Physics Letters, 2020, 116, 061105.	3.3	6
76	Ion Pairing and Redissociaton in Low-Permittivity Electrolytes for Multivalent Battery Applications. Journal of Physical Chemistry Letters, 2020, 11, 2046-2052.	4.6	28
77	Butyltin Keggin Ion with a Rare Four-Coordinate Ca Center. Inorganic Chemistry, 2020, 59, 2900-2909.	4.0	9
78	Aromaticity as a Guide to Planarity in Conjugated Molecules and Polymers. Journal of Physical Chemistry C, 2020, 124, 5608-5612.	3.1	11
79	Uncharted Waters: Super-Concentrated Electrolytes. Joule, 2020, 4, 69-100.	24.0	305
80	From Waste-Heat Recovery to Refrigeration: Compositional Tuning of Magnetocaloric Mn_{1+x}Sb. Chemistry of Materials, 2020, 32, 1243-1249.	6.7	18
81	propnet: A Knowledge Graph for Materials Science. Matter, 2020, 2, 464-480.	10.0	34
82	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
83	Wide Band Gap Chalcogenide Semiconductors. Chemical Reviews, 2020, 120, 4007-4055.	47.7	246
84	Trigonal polymorph of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Li</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Mn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2020, 4, .	2.4	2
85	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
86	Rationalizing Calcium Electrodeposition Behavior by Quantifying Ethereal Solvation Effects on Ca²⁺ Coordination in Well-Dissociated Electrolytes. Journal of the Electrochemical Society, 2020, 167, 160512.	2.9	16
87	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
88	Combining theory and experiment in lithiumâ€“sulfur batteries: Current progress and future perspectives. Materials Today, 2019, 22, 142-158.	14.2	301
89	High-throughput computation and evaluation of raman spectra. Scientific Data, 2019, 6, 135.	5.3	13
90	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

#	Article	IF	Citations
91	High-throughput Computational Study of Halide Double Perovskite Inorganic Compounds. Chemistry of Materials, 2019, 31, 5392-5401.	6.7	102
92	Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 2019, 571, 95-98.	27.8	590
93	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
94	Unraveling the Nanoscale Heterogeneity of Solid Electrolyte Interphase Using Tip-Enhanced Raman Spectroscopy. Joule, 2019, 3, 2001-2019.	24.0	99
95	Transport in Superconcentrated LiPF₆ and LiBF₄/Propylene Carbonate Electrolytes. ACS Energy Letters, 2019, 4, 2843-2849.	17.4	71
96	Ion Association Constants for Lithium Ion Battery Electrolytes from First-Principles Quantum Chemistry. Journal of the Electrochemical Society, 2019, 166, A3554-A3558.	2.9	5
97	Combinatorial Tuning of Structural and Optoelectronic Properties in Cu Zn1â^'S. Matter, 2019, 1, 862-880.	10.0	26
98	Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery. Nature Communications, 2019, 10, 443.	12.8	125
99	The existence and impact of persistent ferroelectric domains in MAPbI ₃. Science Advances, 2019, 5, eaas9311.	10.3	77
100	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
101	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
102	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	5.3	201
103	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
104	Anisotropic work function of elemental crystals. Surface Science, 2019, 687, 48-55.	1.9	84
105	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
106	Materials design of perovskite solid solutions for thermochemical applications. Energy and Environmental Science, 2019, 12, 1369-1384.	30.8	122
107	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
108	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

#	Article	IF	Citations
109	An Electrifying Choice for the 2019 Chemistry Nobel Prize: Goodenough, Whittingham, and Yoshino. Chemistry of Materials, 2019, 31, 8577-8581.	6.7	31
110	Efficient Pourbaix diagrams of many-element compounds. Physical Chemistry Chemical Physics, 2019, 21, 25323-25327.	2.8	69
111	Alkyltin Keggin clusters as EUVL photoresist technology. , 2019, , .		1
112	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
113	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
114	Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite-Size Ion Models. Journal of Physical Chemistry Letters, 2018, 9, 628-634.	4.6	16
115	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
116	High-throughput density-functional perturbation theory phonons for inorganic materials. Scientific Data, 2018, 5, 180065.	5.3	122
117	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€"A Review. Topics in Current Chemistry, 2018, 376, 19.	5.8	61
118	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
119	Thermodynamic limit for synthesis of metastable inorganic materials. Science Advances, 2018, 4, eaaq0148.	10.3	212
120	Automated generation and ensemble-learned matching of X-ray absorption spectra. Npj Computational Materials, 2018, 4, .	8.7	82
121	Efficient Discovery of Optimal N-Layered TMDC Hetero-Structures. MRS Advances, 2018, 3, 397-402.	0.9	5
122	Active learning for accelerated design of layered materials. Npj Computational Materials, 2018, 4, .	8.7	107
123	Garnet Electrolyte Surface Degradation and Recovery. ACS Applied Energy Materials, 2018, 1, 7244-7252.	5.1	81
124	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
125	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
126	Alleviating oxygen evolution from Li-excess oxide materials through theory-guided surface protection. Nature Communications, 2018, 9, 4597.	12.8	56

#	Article	IF	Citations
127	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
128	Assessing High-Throughput Descriptors for Prediction of Transparent Conductors. Chemistry of Materials, 2018, 30, 8375-8389.	6.7	60
129	Mechanical Properties and Chemical Reactivity of Li_xSiO_y Thin Films. ACS Applied Materials & Interfaces, 2018, 10, 38558-38564.	8.0	21
130	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
131	Matminer: An open source toolkit for materials data mining. Computational Materials Science, 2018, 152, 60-69.	3.0	446
132	Alkyltin clusters: the less symmetric Keggin isomers. Dalton Transactions, 2018, 47, 9804-9813.	3.3	31
133	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
134	Evaluation of thermodynamic equations of state across chemistry and structure in the materials project. Npj Computational Materials, 2018, 4, .	8.7	32
135	Elucidating Solvation Structures for Rational Design of Multivalent Electrolytesâ€”A Review. Topics in Current Chemistry Collections, 2018, , 79-124.	0.5	14
136	High-throughput computational X-ray absorption spectroscopy. Scientific Data, 2018, 5, 180151.	5.3	94
137	Ab initio calculation of thermal expansion with application to understanding Invar behavior in gum metal. Physical Review Materials, 2018, 2, .	2.4	2
138	High-throughput screening of inorganic compounds for the discovery of novel dielectric and optical materials. Scientific Data, 2017, 4, 160134.	5.3	140
139	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
140	Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. Chemical Reviews, 2017, 117, 4287-4341.	47.7	914
141	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
142	Group additivity-Pourbaix diagrams advocate thermodynamically stable nanoscale clusters in aqueous environments. Nature Communications, 2017, 8, 15852.	12.8	27
143	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. Npj Computational Materials, 2017, 3, .	8.7	145
144	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

#	Article	IF	Citations
145	A high-throughput framework for determining adsorption energies on solid surfaces. Npj Computational Materials, 2017, 3, .	8.7	70
146	Effects of Anion Mobility on Electrochemical Behaviors of Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
147	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
148	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
149	Computational prediction of new auxetic materials. Nature Communications, 2017, 8, 323.	12.8	105
150	Computational Design of New Magnesium Electrolytes with Improved Properties. Journal of Physical Chemistry C, 2017, 121, 16126-16136.	3.1	26
151	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
152	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
153	Fast Mg2+ diffusion in Mo3(PO4)3O for Mg batteries. Chemical Communications, 2017, 53, 7998-8001.	4.1	22
154	Creation of an XAS and EELS Spectroscopy Resource within the Materials Project using FEFF9. Microscopy and Microanalysis, 2017, 23, 208-209.	0.4	3
155	Predicting defect behavior in B2 intermetallics by merging ab initio modeling and machine learning. Npj Computational Materials, 2016, 2, .	8.7	90
156	Research Update: The materials genome initiative: Data sharing and the impact of collaborative ab initio databases. APL Materials, 2016, 4, .	5.1	115
157	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
158	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
159	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
160	Strain-Mediated Interfacial Dynamics during Auâ€“PbS Coreâ€“Shell Nanostructure Formation. ACS Nano, 2016, 10, 6235-6240.	14.6	21
161	A high capacity thiospinel cathode for Mg batteries. Energy and Environmental Science, 2016, 9, 2273-2277.	30.8	349
162	Materials science with large-scale data and informatics: Unlocking new opportunities. MRS Bulletin, 2016, 41, 399-409.	3.5	192

#	Article	IF	Citations
163	Computational Approach for Epitaxial Polymorph Stabilization through Substrate Selection. ACS Applied Materials & Interfaces, 2016, 8, 13086-13093.	8.0	78
164	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
165	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. Energy and Environmental Science, 2016, 9, 3201-3209.	30.8	121
166	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
167	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
168	Computational predictions of energy materials using density functional theory. Nature Reviews Materials, 2016, 1, .	48.7	536
169	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
170	The thermodynamic scale of inorganic crystalline metastability. Science Advances, 2016, 2, e1600225.	10.3	565
171	Preferential Solvation of an Asymmetric Redox Molecule. Journal of Physical Chemistry C, 2016, 120, 27834-27839.	3.1	18
172	Surface energies of elemental crystals. Scientific Data, 2016, 3, 160080.	5.3	583
173	â€œRocking-Chairâ€•Type Metal Hybrid Supercapacitors. ACS Applied Materials & Interfaces, 2016, 8, 30853-30862.	8.0	86
174	Mechanistic insights into chemical and photochemical transformations of bismuth vanadate photoanodes. Nature Communications, 2016, 7, 12012.	12.8	231
175	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
176	Origin of Electrochemical, Structural, and Transport Properties in Nonaqueous Zinc Electrolytes. ACS Applied Materials & Interfaces, 2016, 8, 3021-3031.	8.0	181
177	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
178	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
179	Revealing the Intrinsic Li Mobility in the Li₂MnO₃ Lithium-Excess Material. Chemistry of Materials, 2016, 28, 2081-2088.	6.7	59
180	Dynamic Control of Optical Response in Layered Metal Chalcogenide Nanoplates. Nano Letters, 2016, 16, 488-496.	9.1	26

#	Article	IF	Citations
181	A Community Contribution Framework for Sharing Materials Data with Materials Project. , 2015, , .		10
182	A database to enable discovery and design of piezoelectric materials. Scientific Data, 2015, 2, 150053.	5.3	191
183	Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
184	FireWorks: a dynamic workflow system designed for highâ€throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
185	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
186	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
187	Effect of Surface Microstructure on Electrochemical Performance of Garnet Solid Electrolytes. ACS Applied Materials & Interfaces, 2015, 7, 2073-2081.	8.0	347
188	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
189	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	19.5	61
190	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
191	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
192	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
193	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
194	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
195	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
196	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. Chemistry of Materials, 2015, 27, 6016-6021.	6.7	445
197	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
198	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

#	Article	IF	Citations
199	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24
200	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
201	Solvation structure and energetics of electrolytes for multivalent energy storage. Physical Chemistry Chemical Physics, 2014, 16, 21941-21945.	2.8	124
202	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
203	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
204	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. Computational Materials Science, 2013, 68, 314-319.	3.0	2,392
205	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 2013, 1, .	5.1	6,913
206	First principles high throughput screening of oxynitrides for water-splitting photocatalysts. Energy and Environmental Science, 2013, 6, 157-168.	30.8	290
207	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
208	Revealing the coupled cation interactions behind the electrochemical profile of LixNi0.5Mn1.5O4. Energy and Environmental Science, 2012, 5, 6047.	30.8	67
209	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
210	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
211	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
212	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
213	Predicting Crystal Structures with Data Mining of Quantum Calculations. Physical Review Letters, 2003, 91, 135503.	7.8	354