

# Gerbrand Ceder

## List of Publications by Year in descending order

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280  
papers

61,772  
citations

1040

113  
h-index

849

244  
g-index

286  
all docs

286  
docs citations

286  
times ranked

36385  
citing authors

#	ARTICLE	IF	CITATIONS
1	Expanding the Ambient-Pressure Phase Space of $\text{CaFe}_2\text{O}_4$ -Type Sodium Postspinel Host-Guest Compounds. <i>ACS Organic &amp; Inorganic Au</i> , 2022, 2, 8-22.	1.9	5
2	Intercalation of Ca into a Highly Defective Manganese Oxide at Room Temperature. <i>Chemistry of Materials</i> , 2022, 34, 836-846.	3.2	10
3	Lithium superionic conductors with corner-sharing frameworks. <i>Nature Materials</i> , 2022, 21, 924-931.	13.3	67
4	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science. <i>Patterns</i> , 2022, 3, 100488.	3.1	46
5	Solid-State Calcium-Ion Diffusion in $\text{Ca}_{1.5}\text{Ba}_{0.5}\text{Si}_5\text{O}_3\text{N}_6$ . <i>Chemistry of Materials</i> , 2022, 34, 128-139.	3.2	7
6	Thermodynamically Driven Synthetic Optimization for Cation-Disordered Rock Salt Cathodes. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	20
7	ULSA: unified language of synthesis actions for the representation of inorganic synthesis protocols. , 2022, 1, 313-324.		10
8	Impact of processing conditions on the film formation of lead-free halide double perovskite $\text{Cs}_2\text{AgBiBr}_6$ . <i>Journal of Materials Chemistry A</i> , 2022, 10, 19868-19880.	5.2	12
9	Dataset of solution-based inorganic materials synthesis procedures extracted from the scientific literature. <i>Scientific Data</i> , 2022, 9, .	2.4	23
10	Text-mined dataset of gold nanoparticle synthesis procedures, morphologies, and size entities. <i>Scientific Data</i> , 2022, 9, .	2.4	24
11	Approaches for handling high-dimensional cluster expansions of ionic systems. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	10
12	Cation-disordered rocksalt-type high-entropy cathodes for Li-ion batteries. <i>Nature Materials</i> , 2021, 20, 214-221.	13.3	290
13	Promises and Challenges of Next-Generation "Beyond Li-ion" Batteries for Electric Vehicles and Grid Decarbonization. <i>Chemical Reviews</i> , 2021, 121, 1623-1669.	23.0	769
14	Computational and experimental search for potential polyanionic K-ion cathode materials. <i>Journal of Materials Chemistry A</i> , 2021, 9, 18564-18575.	5.2	15
15	Toward autonomous design and synthesis of novel inorganic materials. <i>Materials Horizons</i> , 2021, 8, 2169-2198.	6.4	61
16	Opportunities and challenges of text mining in materials research. <i>IScience</i> , 2021, 24, 102155.	1.9	81
17	Manufacturing scalability implications of materials choice in inorganic solid-state batteries. <i>Joule</i> , 2021, 5, 564-580.	11.7	33
18	Fluorination-Enhanced Surface Stability of Cation-Disordered Rocksalt Cathodes for Li-Ion Batteries. <i>Advanced Functional Materials</i> , 2021, 31, 2101888.	7.8	28

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19	Atomic Structure of Surface-Densified Phases in Ni-Rich Layered Compounds. ACS Applied Materials & Interfaces, 2021, 13, 17478-17486.	4.0	13
20	Insights into Layered Oxide Cathodes for Rechargeable Batteries. Molecules, 2021, 26, 3173.	1.7	16
21	Na Redistribution-Induced By K Intercalation during Na/K Ion Exchange in a Layered Oxide Cathode. ECS Meeting Abstracts, 2021, MA2021-01, 358-358.	0.0	0
22	Observing and Modeling the Sequential Pairwise Reactions that Drive Solid-State Ceramic Synthesis. Advanced Materials, 2021, 33, e2100312.	11.1	51
23	Probabilistic Deep Learning Approach to Automate the Interpretation of Multi-phase Diffraction Spectra. Chemistry of Materials, 2021, 33, 4204-4215.	3.2	45
24	Non-topotactic reactions enable high rate capability in Li-rich cathode materials. Nature Energy, 2021, 6, 706-714.	19.8	65
25	Dynamic Barriers to Crystallization of Calcium Barium Carbonates. Crystal Growth and Design, 2021, 21, 4556-4563.	1.4	5
26	Operando X-ray Diffraction Studies of the Mg-Ion Migration Mechanisms in Spinel Cathodes for Rechargeable Mg-Ion Batteries. Journal of the American Chemical Society, 2021, 143, 10649-10658.	6.6	24
27	Toward the Development of a High-Voltage Mg Cathode Using a Chromium Sulfide Host. , 2021, 3, 1213-1220.		12
28	Online Interactive Platform for COVID-19 Literature Visual Analytics: Platform Development Study. Journal of Medical Internet Research, 2021, 23, e26995.	2.1	2
29	Lithium Oxide Superionic Conductors Inspired by Garnet and NASICON Structures. Advanced Energy Materials, 2021, 11, 2101437.	10.2	33
30	Synthetic accessibility and stability rules of NASICONs. Nature Communications, 2021, 12, 5752.	5.8	47
31	Kinetic origins of the metastable zone width in the manganese oxide Pourbaix diagram. Journal of Materials Chemistry A, 2021, 9, 7857-7867.	5.2	7
32	Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes. Matter, 2021, 4, 3897-3916.	5.0	32
33	Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic First-Principles Evaluation. Advanced Energy Materials, 2021, 11, 2101698.	10.2	8
34	(Invited) Novel Approaches for the Study of Disordered Rocksalt Oxyfluoride Intercalation Cathodes. ECS Meeting Abstracts, 2021, MA2021-02, 190-190.	0.0	0
35	(Invited) From Layered Oxides to Disordered Rocksalt Cathodes: The Role of Electronic Structure, Cation Order, and Structure on the Performance of Dense Cathode Materials. ECS Meeting Abstracts, 2021, MA2021-02, 184-184.	0.0	0
36	Sparse expansions of multicomponent oxide configuration energy using coherency and redundancy. Physical Review B, 2021, 104, .	1.1	9

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37	Design Principles for High-Capacity Mn-Based Cation-Disordered Rocksalt Cathodes. <i>CheM</i> , 2020, 6, 153-168.	5.8	103
38	All-Solid-State Batteries: High Active Material Loading in All-Solid-State Battery Electrode via Particle Size Optimization ( <i>Adv. Energy Mater.</i> 1/2020). <i>Advanced Energy Materials</i> , 2020, 10, 2070004.	10.2	7
39	Probing Mg Migration in Spinel Oxides. <i>Chemistry of Materials</i> , 2020, 32, 663-670.	3.2	53
40	Understanding interface stability in solid-state batteries. <i>Nature Reviews Materials</i> , 2020, 5, 105-126.	23.3	630
41	High Active Material Loading in All-Solid-State Battery Electrode via Particle Size Optimization. <i>Advanced Energy Materials</i> , 2020, 10, 1902881.	10.2	152
42	Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ . <i>Chemistry of Materials</i> , 2020, 32, 8981-8992.	3.2	14
43	Increasing Capacity in Disordered Rocksalt Cathodes by Mg Doping. <i>Chemistry of Materials</i> , 2020, 32, 10728-10736.	3.2	21
44	First-principles study of $\text{CaB}_{12}\text{H}_{12}$ as a potential solid-state conductor for Ca. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27600-27604.	1.3	8
45	Kinetic Pathways Templated by Low-Temperature Intermediates during Solid-State Synthesis of Layered Oxides. <i>Chemistry of Materials</i> , 2020, 32, 9906-9913.	3.2	34
46	Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19965-19974.	5.2	20
47	Similarity of Precursors in Solid-State Synthesis as Text-Mined from Scientific Literature. <i>Chemistry of Materials</i> , 2020, 32, 7861-7873.	3.2	49
48	Characterization of mechanical degradation in an all-solid-state battery cathode. <i>Journal of Materials Chemistry A</i> , 2020, 8, 17399-17404.	5.2	100
49	A critical examination of compound stability predictions from machine-learned formation energies. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	119
50	Data-driven materials research enabled by natural language processing and information extraction. <i>Applied Physics Reviews</i> , 2020, 7, .	5.5	117
51	The Impact of Surface Structure Transformations on the Performance of Li-Excess Cation-Disordered Rocksalt Cathodes. <i>Cell Reports Physical Science</i> , 2020, 1, 100187.	2.8	20
52	The interplay between thermodynamics and kinetics in the solid-state synthesis of layered oxides. <i>Nature Materials</i> , 2020, 19, 1088-1095.	13.3	129
53	Direct Visualization of the Interfacial Degradation of Cathode Coatings in Solid State Batteries: A Combined Experimental and Computational Study. <i>Advanced Energy Materials</i> , 2020, 10, 1903778.	10.2	67
54	Energy storage emerging: A perspective from the Joint Center for Energy Storage Research. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 12550-12557.	3.3	218

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55	Ultrahigh power and energy density in partially ordered lithium-ion cathode materials. <i>Nature Energy</i> , 2020, 5, 213-221.	19.8	158
56	Direct Observation of Alternating Octahedral and Prismatic Sodium Layers in O <sub>3</sub> -Type Transition Metal Oxides. <i>Advanced Energy Materials</i> , 2020, 10, 2001151.	10.2	39
57	Electrodeposition and Mechanical Stability at Lithium-Solid Electrolyte Interface during Plating in Solid-State Batteries. <i>Cell Reports Physical Science</i> , 2020, 1, 100106.	2.8	77
58	An Analysis of Solid-State Electrodeposition-Induced Metal Plastic Flow and Predictions of Stress States in Solid Ionic Conductor Defects. <i>Journal of the Electrochemical Society</i> , 2020, 167, 020534.	1.3	49
59	Kinetic pathways of ionic transport in fast-charging lithium titanate. <i>Science</i> , 2020, 367, 1030-1034.	6.0	197
60	Perspectives on Cobalt Supply through 2030 in the Face of Changing Demand. <i>Environmental Science &amp; Technology</i> , 2020, 54, 2985-2993.	4.6	116
61	Selective metathesis synthesis of MgCr <sub>2</sub> S <sub>4</sub> by control of thermodynamic driving forces. <i>Materials Horizons</i> , 2020, 7, 1310-1316.	6.4	27
62	Computational Investigation of Halogen-Substituted Na Argyrodites as Solid-State Superionic Conductors. <i>Chemistry of Materials</i> , 2020, 32, 1896-1903.	3.2	9
63	Effect of Fluorination on Lithium Transport and Short-Range Order in Disordered-Rocksalt-Type Lithium-Ion Battery Cathodes. <i>Advanced Energy Materials</i> , 2020, 10, 1903240.	10.2	83
64	Na <sup>+</sup> Redistribution by Electrochemical Na <sup>+</sup> /K <sup>+</sup> Exchange in Layered Na <sub>x</sub> Ni <sub>2</sub> SbO <sub>6</sub> . <i>Chemistry of Materials</i> , 2020, 32, 4312-4323.	3.2	14
65	A High-Energy NASICON-Type Cathode Material for Na-Ion Batteries. <i>Advanced Energy Materials</i> , 2020, 10, 1903968.	10.2	116
66	Origin of Capacity Degradation of High-Voltage KVPO <sub>4</sub> F Cathode. <i>Journal of the Electrochemical Society</i> , 2020, 167, 110555.	1.3	22
67	(Invited) Complex Phase Transitions in Layered Sodium Transition Metal Oxides. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 519-519.	0.0	0
68	The Interplay between Thermodynamics and Kinetics in the Solid-State Synthesis of Layered Oxides. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 313-313.	0.0	0
69	Understanding Metal Deposition in Solid Electrolytes Due to Mixed Ionic-Electronic Conduction. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 972-972.	0.0	0
70	High-Entropy-Type Cation-Disordered Rocksalt Cathodes for Li-Ion Batteries with Enhanced Capacity and Rate Capability. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 3796-3796.	0.0	0
71	(Keynote) Chemical and Mechanical Stability Issues at Electrolyte/Electrode Interfaces in Solid State Batteries. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 954-954.	0.0	0
72	Investigation of Rare-Earth Chalcogenide Spinel for Mg Solid State Conductors. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 234-234.	0.0	0

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73	(Invited) How Does Intercalation Ion Species Determine the Electrochemical Properties of Cathode Materials for Rechargeable Batteries?. ECS Meeting Abstracts, 2020, MA2020-02, 169-169.	0.0	0
74	Short-Range Order and Macroscopic Lithium Transport in Cation-Disordered Rocksalt Cathodes. ECS Meeting Abstracts, 2020, MA2020-02, 75-75.	0.0	0
75	Thermodynamics of Spinel-like Cation Partial Ordering in Ultrahigh Power and Energy Density Li-Ion Batteries for Fast-Charging Electric Vehicles. ECS Meeting Abstracts, 2020, MA2020-02, 622-622.	0.0	0
76	Resolving Li-F Locking Effect in Disordered Rocksalt Cathodes with Mg-Doping. ECS Meeting Abstracts, 2020, MA2020-02, 129-129.	0.0	0
77	Kinetic Pathways of Ionic Transport in Fast Charging Lithium Titanate. ECS Meeting Abstracts, 2020, MA2020-02, 546-546.	0.0	0
78	Ultrahigh Power and Energy Density in Partially Ordered Lithium-Ion Cathode Materials. ECS Meeting Abstracts, 2020, MA2020-02, 153-153.	0.0	0
79	Rationalizing accurate structure prediction in the meta-GGA SCAN functional. Physical Review B, 2019, 100, .	1.1	56
80	Semi-supervised machine-learning classification of materials synthesis procedures. Npj Computational Materials, 2019, 5, .	3.5	85
81	Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 2019, 571, 95-98.	13.7	590
82	Text-mined dataset of inorganic materials synthesis recipes. Scientific Data, 2019, 6, 203.	2.4	121
83	Reactivity-Guided Interface Design in Na Metal Solid-State Batteries. Joule, 2019, 3, 1037-1050.	11.7	120
84	Metal-oxygen decoordination stabilizes anion redox in Li-rich oxides. Nature Materials, 2019, 18, 256-265.	13.3	280
85	A map of the inorganic ternary metal nitrides. Nature Materials, 2019, 18, 732-739.	13.3	274
86	Investigation of Alkali-ion (Li, Na, and K) Intercalation in $K_{x}VPO_{4}F$ ( $x \approx 1/4$ ) Cathode. Advanced Functional Materials, 2019, 29, 1902392.	7.8	35
87	Distilling a Materials Synthesis Ontology. Matter, 2019, 1, 8-12.	5.0	31
88	Next-Generation Cathode Materials for Non-aqueous Potassium-Ion Batteries. Trends in Chemistry, 2019, 1, 682-692.	4.4	70
89	$Zn_{2}SbN_{3}$ : growth and characterization of a metastable photoactive semiconductor. Materials Horizons, 2019, 6, 1669-1674.	6.4	32
90	Computational Screening of Cathode Coatings for Solid-State Batteries. Joule, 2019, 3, 1252-1275.	11.7	276

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91	Computational Investigation and Experimental Realization of Disordered High-Capacity Li-Ion Cathodes Based on Ni Redox. <i>Chemistry of Materials</i> , 2019, 31, 2431-2442.	3.2	50
92	Hidden structural and chemical order controls lithium transport in cation-disordered oxides for rechargeable batteries. <i>Nature Communications</i> , 2019, 10, 592.	5.8	162
93	Evaluation of Mg Compounds as Coating Materials in Mg Batteries. <i>Frontiers in Chemistry</i> , 2019, 7, 24.	1.8	46
94	Non-equilibrium crystallization pathways of manganese oxides in aqueous solution. <i>Nature Communications</i> , 2019, 10, 573.	5.8	66
95	<i>Ab initio</i> investigation of the stability of electrolyte/electrode interfaces in all-solid-state Na batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 8144-8155.	5.2	102
96	Understanding Surface Densified Phases in Ni-Rich Layered Compounds. <i>ACS Energy Letters</i> , 2019, 4, 811-818.	8.8	64
97	Improved Cycling Performance of Li-Excess Cation-Disordered Cathode Materials upon Fluorine Substitution. <i>Advanced Energy Materials</i> , 2019, 9, 1802959.	10.2	127
98	Synthesis and Electrochemical Properties of $\text{Li}_{1+2x}\text{Zn}_{1-x}\text{PS}_4$ -Type Solid Electrolyte. <i>Chemistry of Materials</i> , 2018, 30, 2236-2244.	3.2	30
99	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. <i>Journal of the American Chemical Society</i> , 2018, 140, 4293-4301.	6.6	53
100	The effect of surface-bulk potential difference on the kinetics of intercalation in core-shell active cathode particles. <i>Journal of Power Sources</i> , 2018, 382, 30-37.	4.0	7
101	On the Balance of Intercalation and Conversion Reactions in Battery Cathodes. <i>Advanced Energy Materials</i> , 2018, 8, 1800379.	10.2	43
102	Reversible $\text{Mn}^{2+}/\text{Mn}^{4+}$ double redox in lithium-excess cathode materials. <i>Nature</i> , 2018, 556, 185-190.	13.7	525
103	Localized concentration reversal of lithium during intercalation into nanoparticles. <i>Science Advances</i> , 2018, 4, eaao2608.	4.7	50
104	Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite-Size Ion Models. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 628-634.	2.1	16
105	Constructing first-principles phase diagrams of amorphous $\text{Li}_x\text{Si}$ using machine-learning-assisted sampling with an evolutionary algorithm. <i>Journal of Chemical Physics</i> , 2018, 148, 241711.	1.2	121
106	Efficient first-principles prediction of solid stability: Towards chemical accuracy. <i>Npj Computational Materials</i> , 2018, 4, .	3.5	157
107	Fluorination of Lithium-Excess Transition Metal Oxide Cathode Materials. <i>Advanced Energy Materials</i> , 2018, 8, 1701533.	10.2	115
108	First-Principles Study of the Voltage Profile and Mobility of Mg Intercalation in a Chromium Oxide Spinel. <i>Chemistry of Materials</i> , 2018, 30, 153-162.	3.2	53

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109	Recent Progress and Perspective in Electrode Materials for $\text{K}^{\ominus}$ Batteries. <i>Advanced Energy Materials</i> , 2018, 8, 1702384.	10.2	549
110	Shear-Assisted Formation of Cation-Disordered Rocksalt $\text{NaMO}_2$ (M = Fe or Mn). <i>Chemistry of Materials</i> , 2018, 30, 8811-8821.	3.2	17
111	Understanding Crystallization Pathways of $\text{MnO}_x$ Polymorph Formation via in-situ X-ray Scattering. <i>Microscopy and Microanalysis</i> , 2018, 24, 1486-1487.	0.2	1
112	Predictive modeling and design rules for solid electrolytes. <i>MRS Bulletin</i> , 2018, 43, 746-751.	1.7	47
113	Structural and Compositional Factors That Control the Li-Ion Conductivity in LiPON Electrolytes. <i>Chemistry of Materials</i> , 2018, 30, 7077-7090.	3.2	105
114	Short-Range Order and Unusual Modes of Nickel Redox in a Fluorine-Substituted Disordered Rocksalt Oxide Lithium-Ion Cathode. <i>Chemistry of Materials</i> , 2018, 30, 6945-6956.	3.2	72
115	Deposition and Stripping Behavior of Lithium Metal in Electrochemical System: Continuum Mechanics Study. <i>Chemistry of Materials</i> , 2018, 30, 6769-6776.	3.2	74
116	Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries. <i>Chemistry of Materials</i> , 2018, 30, 6532-6539.	3.2	108
117	Electrochemical trapping of metastable $\text{Mn}^{3+}$ ions for activation of $\text{MnO}_2$ oxygen evolution catalysts. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E5261-E5268.	3.3	173
118	Design principles for high transition metal capacity in disordered rocksalt Li-ion cathodes. <i>Energy and Environmental Science</i> , 2018, 11, 2159-2171.	15.6	123
119	Understanding crystallization pathways leading to manganese oxide polymorph formation. <i>Nature Communications</i> , 2018, 9, 2553.	5.8	98
120	A First-Principles and Experimental Investigation of Nickel Solubility into the $\text{P2 Na}_x\text{CoO}_2$ Sodium-Ion Cathode. <i>Advanced Energy Materials</i> , 2018, 8, 1801446.	10.2	34
121	A New Strategy for High-Voltage Cathodes for $\text{K}^{\ominus}$ Batteries: Stoichiometric $\text{KVPO}_4$ . <i>Advanced Energy Materials</i> , 2018, 8, 1801591.	10.2	130
122	Revealing and Rationalizing the Rich Polytypism of Todorokite $\text{MnO}_2$ . <i>Journal of the American Chemical Society</i> , 2018, 140, 6961-6968.	6.6	36
123	Electrochemical properties and structural evolution of $\text{O}_3$ -type layered sodium mixed transition metal oxides with trivalent nickel. <i>Journal of Materials Chemistry A</i> , 2017, 5, 4596-4606.	5.2	63
124	Thermodynamics of Phase Selection in $\text{MnO}_2$ Framework Structures through Alkali Intercalation and Hydration. <i>Journal of the American Chemical Society</i> , 2017, 139, 2672-2681.	6.6	158
125	Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. <i>Chemical Reviews</i> , 2017, 117, 4287-4341.	23.0	914
126	Magnesium ion mobility in post-spinels accessible at ambient pressure. <i>Chemical Communications</i> , 2017, 53, 5171-5174.	2.2	21

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127	Additional Sodium Insertion into Polyanionic Cathodes for Higher-Energy Na-Ion Batteries. <i>Advanced Energy Materials</i> , 2017, 7, 1700514.	10.2	157
128	K-Ion Batteries Based on a P2-Type $K_{0.6}CoO_2$ Cathode. <i>Advanced Energy Materials</i> , 2017, 7, 1700098.	10.2	250
129	Compatibility issues between electrodes and electrolytes in solid-state batteries. <i>Energy and Environmental Science</i> , 2017, 10, 1150-1166.	15.6	267
130	Electrolyte-Induced Surface Transformation and Transition-Metal Dissolution of Fully Delithiated $Li_{0.8}Co_{0.15}Al_{0.05}O_2$ . <i>Langmuir</i> , 2017, 33, 9333-9353.	1.6	70
131	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. <i>Npj Computational Materials</i> , 2017, 3, .	3.5	145
132	Electronic-Structure Origin of Cation Disorder in Transition-Metal Oxides. <i>Physical Review Letters</i> , 2017, 119, 176402.	2.9	135
133	Lithium-Ion Battery Supply Chain Considerations: Analysis of Potential Bottlenecks in Critical Metals. <i>Joule</i> , 2017, 1, 229-243.	11.7	937
134	Mitigating oxygen loss to improve the cycling performance of high capacity cation-disordered cathode materials. <i>Nature Communications</i> , 2017, 8, 981.	5.8	197
135	Materials Synthesis Insights from Scientific Literature via Text Extraction and Machine Learning. <i>Chemistry of Materials</i> , 2017, 29, 9436-9444.	3.2	319
136	Influence of Inversion on Mg Mobility and Electrochemistry in Spinel. <i>Chemistry of Materials</i> , 2017, 29, 7918-7930.	3.2	75
137	First-Principles Simulation of the $(Li-Ni-Vacancy)O$ Phase Diagram and Its Relevance for the Surface Phases in Ni-Rich Li-Ion Cathode Materials. <i>Chemistry of Materials</i> , 2017, 29, 7840-7851.	3.2	79
138	Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species. <i>Physical Review B</i> , 2017, 96, .	1.1	228
139	Induction time of a polymorphic transformation. <i>CrystEngComm</i> , 2017, 19, 4576-4585.	1.3	43
140	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. <i>Chemistry of Materials</i> , 2017, 29, 6936-6946.	3.2	121
141	Computational Prediction and Evaluation of Solid-State Sodium Superionic Conductors $Na_7P_3X_{11}$ ( $X = O, S, Se$ ). <i>Chemistry of Materials</i> , 2017, 29, 7475-7482.	3.2	56
142	Investigation of Potassium Storage in Layered P3-Type $K_{0.5}MnO_2$ Cathode. <i>Advanced Materials</i> , 2017, 29, 1702480.	11.1	268
143	Construction of ground-state preserving sparse lattice models for predictive materials simulations. <i>Npj Computational Materials</i> , 2017, 3, .	3.5	15
144	Communication: O3-Type Layered Oxide with a Quaternary Transition Metal Composition for Na-Ion Battery Cathodes: $NaTi_{0.25}Fe_{0.25}Co_{0.25}Ni_{0.25}O_2$ . <i>Journal of the Electrochemical Society</i> , 2017, 164, A3484-A3486.	1.3	16

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145	High-fraction brookite films from amorphous precursors. <i>Scientific Reports</i> , 2017, 7, 15232.	1.6	56
146	Fast Mg <sup>2+</sup> diffusion in Mo <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> O for Mg batteries. <i>Chemical Communications</i> , 2017, 53, 7998-8001.	2.2	22
147	High magnesium mobility in ternary spinel chalcogenides. <i>Nature Communications</i> , 2017, 8, 1759.	5.8	212
148	Computational Design and Preparation of Cation-Disordered Oxides for High-Energy-Density Li-Ion Batteries. <i>Advanced Energy Materials</i> , 2016, 6, 1600488.	10.2	93
149	Evaluating structure selection in the hydrothermal growth of FeS <sub>2</sub> pyrite and marcasite. <i>Nature Communications</i> , 2016, 7, 13799.	5.8	67
150	An efficient algorithm for finding the minimum energy path for cation migration in ionic materials. <i>Journal of Chemical Physics</i> , 2016, 145, 074112.	1.2	54
151	A high capacity thiospinel cathode for Mg batteries. <i>Energy and Environmental Science</i> , 2016, 9, 2273-2277.	15.6	349
152	Structural and Na-ion conduction characteristics of Na <sub>3</sub> PS <sub>4</sub> Se <sub>4</sub> . <i>Journal of Materials Chemistry A</i> , 2016, 4, 9044-9053.	5.2	73
153	A bio-facilitated synthetic route for nano-structured complex electrode materials. <i>Green Chemistry</i> , 2016, 18, 2619-2624.	4.6	16
154	The Effect of Cation Disorder on the Average Li Intercalation Voltage of Transition-Metal Oxides. <i>Chemistry of Materials</i> , 2016, 28, 3659-3665.	3.2	62
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