Gerbrand Ceder

List of Publications by Citations

Source: https://exaly.com/author-pdf/2048050/gerbrand-ceder-publications-by-citations.pdf
Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

259 papers	44,349 citations	98 h-index	210 g-index
286 ext. papers	52,687 ext. citations	14.3 avg, IF	8 L-index

#	Paper	IF	Citations
259	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. *APL Materials*, **2013**, 1, 011002	5.7	4073
258	Battery materials for ultrafast charging and discharging. *Nature*, **2009**, 458, 190-3	50.4	2837
257	Electrode Materials for Rechargeable Sodium-Ion Batteries: Potential Alternatives to Current Lithium-Ion Batteries. *Advanced Energy Materials*, **2012**, 2, 710-721	21.8	2590
256	Electrodes with high power and high capacity for rechargeable lithium batteries. *Science*, **2006**, 311, 977-80	39.3	2120
255	Oxidation energies of transition metal oxides within the GGA+U framework. *Physical Review B*, **2006**, 73,	3.3	1568
254	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. *Computational Materials Science*, **2013**, 68, 314-319	3.2	1435
253	Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials. *Energy and Environmental Science*, **2011**, 4, 3680	35.4	1078
252	Design principles for solid-state lithium superionic conductors. *Nature Materials*, **2015**, 14, 1026-31	27	817
251	Interface Stability in Solid-State Batteries. *Chemistry of Materials*, **2016**, 28, 266-273	9.6	792
250	Unlocking the potential of cation-disordered oxides for rechargeable lithium batteries. *Science*, **2014**, 343, 519-22	33.3	722
249	The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials. *Nature Chemistry*, **2016**, 8, 692-7	17.6	713
248	Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. *Chemical Reviews*, **2017**, 117, 4287-4341	68.1	687
247	A high-throughput infrastructure for density functional theory calculations. *Computational Materials Science*, **2011**, 50, 2295-2310	3.2	609
246	Formation enthalpies by mixing GGA and GGA + U calculations. *Physical Review B*, **2011**, 84,	3.3	607
245	Lithium-Ion Battery Supply Chain Considerations: Analysis of Potential Bottlenecks in Critical Metals. *Joule*, **2017**, 1, 229-243	27.8	581
244	Particle size dependence of the ionic diffusivity. *Nano Letters*, **2010**, 10, 4123-7	11.5	544
243	Li_xFePO_4 Phase Diagram from First Principles Calculations. *Chemistry of Materials*, **2008**, 20, 1798-1807	9.6	484

242	First Principles Study of the Li10GeP2S12 Lithium Super Ionic Conductor Material. *Chemistry of Materials*, **2012**, 24, 15-17	9.6	459
241	Electrochemical Properties of Monoclinic NaMnO2. *Journal of the Electrochemical Society*, **2011**, 158, A1307	3.9	450
240	Phase stability, electrochemical stability and ionic conductivity of the Li10±1MP2X12 (M = Ge, Si, Sn, Al or P, and X = O, S or Se) family of superionic conductors. *Energy and Environmental Science*, **2013**, 6, 148-156	35.4	429
239	Charting the complete elastic properties of inorganic crystalline compounds. *Scientific Data*, **2015**, 2, 150009	8.2	428
238	Recent Progress and Perspective in Electrode Materials for K-Ion Batteries. *Advanced Energy Materials*, **2018**, 8, 1702384	21.8	428
237	Finding Nature's Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory. *Chemistry of Materials*, **2010**, 22, 3762-3767	9.6	409
236	Reversible Mn/Mn double redox in lithium-excess cathode materials. *Nature*, **2018**, 556, 185-190	50.4	376
235	Factors that affect Li mobility in layered lithium transition metal oxides. *Physical Review B*, **2006**, 74,	3.3	354
234	The thermodynamic scale of inorganic crystalline metastability. *Science Advances*, **2016**, 2, e1600225	14.3	352
233	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. *Chemistry of Materials*, **2015**, 27, 6016-6021	9.6	351
232	Predicting crystal structure by merging data mining with quantum mechanics. *Nature Materials*, **2006**, 5, 641-6	27	329
231	Spinel compounds as multivalent battery cathodes: a systematic evaluation based on ab initio calculations. *Energy and Environmental Science*, **2015**, 8, 964-974	35.4	326
230	Unsupervised word embeddings capture latent knowledge from materials science literature. *Nature*, **2019**, 571, 95-98	50.4	325
229	Understanding interface stability in solid-state batteries. *Nature Reviews Materials*, **2020**, 5, 105-126	73.3	318
228	Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput ab Initio Calculations. *Chemistry of Materials*, **2011**, 23, 3495-3508	9.6	317
227	Computational understanding of Li-ion batteries. *Npj Computational Materials*, **2016**, 2,	10.9	299
226	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,	3.3	298
225	Ab initio study of the migration of small polarons in olivine LixFePO4 and their association with lithium ions and vacancies. *Physical Review B*, **2006**, 73,	3.3	286

224	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. *Chemistry of Materials*, **2011**, 23, 2979-2986	9.6	271
223	Thermodynamic and kinetic properties of the Li-graphite system from first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	270
222	A high capacity thiospinel cathode for Mg batteries. *Energy and Environmental Science*, **2016**, 9, 2273-2277	35.4	266
221	A Critical Review of the Li Insertion Mechanisms in LiFePO4Electrodes. *Journal of the Electrochemical Society*, **2013**, 160, A3179-A3197	3.9	243
220	Role of electronic structure in the susceptibility of metastable transition-metal oxide structures to transformation. *Chemical Reviews*, **2004**, 104, 4513-33	68.1	242
219	Prediction of solid-aqueous equilibria: Scheme to combine first-principles calculations of solids with experimental aqueous states. *Physical Review B*, **2012**, 85,	3.3	234
218	Data mined ionic substitutions for the discovery of new compounds. *Inorganic Chemistry*, **2011**, 50, 656-663	5.1	230
217	NaTiO2: a layered anode material for sodium-ion batteries. *Energy and Environmental Science*, **2015**, 8, 195-202	35.4	220
216	First principles high throughput screening of oxynitrides for water-splitting photocatalysts. *Energy and Environmental Science*, **2013**, 6, 157-168	35.4	219
215	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	3.2	213
214	K-Ion Batteries Based on a P2-Type K0.6CoO2 Cathode. *Advanced Energy Materials*, **2017**, 7, 1700098	21.8	208
213	Electrochemical Properties of Monoclinic NaNiO2. *Journal of the Electrochemical Society*, **2013**, 160, A207-A211	3.9	206
212	Materials Synthesis Insights from Scientific Literature via Text Extraction and Machine Learning. *Chemistry of Materials*, **2017**, 29, 9436-9444	9.6	202
211	The Configurational Space of Rocksalt-Type Oxides for High-Capacity Lithium Battery Electrodes. *Advanced Energy Materials*, **2014**, 4, 1400478	21.8	197
210	Investigation of Potassium Storage in Layered P3-Type K MnO Cathode. *Advanced Materials*, **2017**, 29, 1702480	24	197
209	Tailoring the Morphology of LiCoO2: A First Principles Study. *Chemistry of Materials*, **2009**, 21, 3799-3809	9.6	197
208	Compatibility issues between electrodes and electrolytes in solid-state batteries. *Energy and Environmental Science*, **2017**, 10, 1150-1166	35.4	196
207	Design and synthesis of the superionic conductor Na10SnP2S12. *Nature Communications*, **2016**, 7, 11009	17.4	193

206	Direct visualization of the Jahn-Teller effect coupled to Na ordering in Na5/8MnO2. *Nature Materials*, **2014**, 13, 586-92	27	191
205	First-Principles Studies on Cation Dopants and Electrolyte|Cathode Interphases for Lithium Garnets. *Chemistry of Materials*, **2015**, 27, 4040-4047	9.6	190
204	Promises and Challenges of Next-Generation "Beyond Li-ion" Batteries for Electric Vehicles and Grid Decarbonization. *Chemical Reviews*, **2021**, 121, 1623-1669	68.1	189
203	Effect of High Voltage on the Structure and Electrochemistry of LiNi0.5Mn0.5O2:□A Joint Experimental and Theoretical Study. *Chemistry of Materials*, **2006**, 18, 4768-4781	9.6	181
202	Metal-oxygen decoordination stabilizes anion redox in Li-rich oxides. *Nature Materials*, **2019**, 18, 256-265	27	178
201	Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations. *Journal of Materials Chemistry*, **2011**, 21, 17147		173
200	A new class of high capacity cation-disordered oxides for rechargeable lithium batteries: Li-Ni-Ti-Mo oxides. *Energy and Environmental Science*, **2015**, 8, 3255-3265	35.4	169
199	First-Principles Evidence for Stage Ordering in Li x CoO2. *Journal of the Electrochemical Society*, **1998**, 145, 2149-2155	3.9	168
198	Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species. *Physical Review B*, **2017**, 96,	3.3	163
197	Computational Screening of Cathode Coatings for Solid-State Batteries. *Joule*, **2019**, 3, 1252-1275	27.8	162
196	High Rate Micron-Sized Ordered LiNi[sub 0.5]Mn[sub 1.5]O[sub 4]. *Journal of the Electrochemical Society*, **2010**, 157, A925	3.9	157
195	O3-type Na(Mn0.25Fe0.25Co0.25Ni0.25)O2: A quaternary layered cathode compound for rechargeable Na ion batteries. *Electrochemistry Communications*, **2014**, 49, 51-54	5.1	156
194	Configurational electronic entropy and the phase diagram of mixed-valence oxides: the case of LixFePO4. *Physical Review Letters*, **2006**, 97, 155704	7.4	155
193	A Facile Mechanism for Recharging Li2O2 in Li-O2 Batteries. *Chemistry of Materials*, **2013**, 25, 3328-3336	9.6	153
192	LiAl y Co1 □y O 2 (R 3 m) Intercalation Cathode for Rechargeable Lithium Batteries. *Journal of the Electrochemical Society*, **1999**, 146, 862-868	3.9	151
191	Synthesis and Stoichiometry of Different Layered Sodium Cobalt Oxides. *Chemistry of Materials*, **2014**, 26, 5288-5296	9.6	150
190	A map of the inorganic ternary metal nitrides. *Nature Materials*, **2019**, 18, 732-739	27	148
189	Energetics of MnO2 polymorphs in density functional theory. *Physical Review B*, **2016**, 93,	3.3	147

188	Role of Structural H2O in Intercalation Electrodes: The Case of Mg in Nanocrystalline Xerogel-V2O5. *Nano Letters*, **2016**, 16, 2426-31	11.5	146
187	A Statistical Learning Framework for Materials Science: Application to Elastic Moduli of k-nary Inorganic Polycrystalline Compounds. *Scientific Reports*, **2016**, 6, 34256	4.9	142
186	Effect of Rb and Ta Doping on the Ionic Conductivity and Stability of the Garnet Li7+2x−y(La3−xRbx)(Zr2−yTay)O12 (0 ≤ x ≤ 0.375, 0 ≤ y ≤ 1) Superionic Conductor: A First Principles Investigation. *Chemistry of Materials*, **2013**, 25, 3048-3055	9.6	140
185	High magnesium mobility in ternary spinel chalcogenides. *Nature Communications*, **2017**, 8, 1759	17.4	137
184	Phase Transitions in the LiNi0.5Mn0.5O2 System with Temperature. *Chemistry of Materials*, **2007**, 19, 1790-1800	9.6	137
183	Mitigating oxygen loss to improve the cycling performance of high capacity cation-disordered cathode materials. *Nature Communications*, **2017**, 8, 981	17.4	136
182	A comparison of destabilization mechanisms of the layered Na(x)MO2 and Li(x)MO2 compounds upon alkali de-intercalation. *Physical Chemistry Chemical Physics*, **2012**, 14, 15571-8	3.6	134
181	Electrochemical trapping of metastable Mn ions for activation of MnO oxygen evolution catalysts. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E5261-E5268	11.5	129
180	Nucleation of metastable aragonite CaCO3 in seawater. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 3199-204	11.5	126
179	S=12 chains and spin-Peierls transition in TiOCl. *Physical Review B*, **2003**, 67,	3.3	125
178	About the Compatibility between High Voltage Spinel Cathode Materials and Solid Oxide Electrolytes as a Function of Temperature. *ACS Applied Materials & Interfaces*, **2016**, 8, 26842-26850	9.5	122
177	Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations. *Chemistry of Materials*, **2014**, 26, 5208-5214	9.6	121
176	First-principles evaluation of multi-valent cation insertion into orthorhombic V2O5. *Chemical Communications*, **2015**, 51, 13619-22	5.8	120
175	Efficient creation and convergence of surface slabs. *Surface Science*, **2013**, 617, 53-59	1.8	120
174	Additional Sodium Insertion into Polyanionic Cathodes for Higher-Energy Na-Ion Batteries. *Advanced Energy Materials*, **2017**, 7, 1700514	21.8	116
173	A disordered rock-salt Li-excess cathode material with high capacity and substantial oxygen redox activity: Li1.25Nb0.25Mn0.5O2. *Electrochemistry Communications*, **2015**, 60, 70-73	5.1	115
172	Thermodynamics of Phase Selection in MnO Framework Structures through Alkali Intercalation and Hydration. *Journal of the American Chemical Society*, **2017**, 139, 2672-2681	16.4	114
171	Screening for high-performance piezoelectrics using high-throughput density functional theory. *Physical Review B*, **2011**, 84,	3.3	108

170	Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries. *Energy and Environmental Science*, **2015**, 8, 3718-3730	35.4	107
169	Efficient first-principles prediction of solid stability: Towards chemical accuracy. *Npj Computational Materials*, **2018**, 4,	10.9	107
168	High-Performance P2-Type Na2/3(Mn1/2Fe1/4Co1/4)O2 Cathode Material with Superior Rate Capability for Na-Ion Batteries. *Advanced Energy Materials*, **2015**, 5, 1500944	21.8	105
167	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	11.5	103
166	Synthesis, computed stability, and crystal structure of a new family of inorganic compounds: carbonophosphates. *Journal of the American Chemical Society*, **2012**, 134, 19619-27	16.4	101
165	The Intercalation Phase Diagram of Mg in V2O5 from First-Principles. *Chemistry of Materials*, **2015**, 27, 3733-3742	9.6	100
164	Layered-to-Rock-Salt Transformation in Desodiated NaxCrO2 (x 0.4). *Chemistry of Materials*, **2016**, 28, 1419-1429	9.6	100
163	Calibrating transition-metal energy levels and oxygen bands in first-principles calculations: Accurate prediction of redox potentials and charge transfer in lithium transition-metal oxides. *Physical Review B*, **2015**, 92,	3.3	98
162	Temperature-concentration phase diagram of P2-NaxCoO2 from first-principles calculations. *Physical Review B*, **2008**, 77,	3.3	98
161	Kinetic pathways of ionic transport in fast-charging lithium titanate. *Science*, **2020**, 367, 1030-1034	33.3	95
160	Effective mass and Fermi surface complexity factor from ab initio band structure calculations. *Npj Computational Materials*, **2017**, 3,	10.9	92
159	Ultrahigh power and energy density in partially ordered lithium-ion cathode materials. *Nature Energy*, **2020**, 5, 213-221	62.3	91
158	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. *Energy and Environmental Science*, **2016**, 9, 3201-3209	35.4	91
157	A New Strategy for High-Voltage Cathodes for K-Ion Batteries: Stoichiometric KVPO4F. *Advanced Energy Materials*, **2018**, 8, 1801591	21.8	90
156	Cation-disordered rocksalt-type high-entropy cathodes for Li-ion batteries. *Nature Materials*, **2021**, 20, 214-221	27	90
155	JahnTeller Assisted Na Diffusion for High Performance Na Ion Batteries. *Chemistry of Materials*, **2016**, 28, 6575-6583	9.6	89
154	High Active Material Loading in All-Solid-State Battery Electrode via Particle Size Optimization. *Advanced Energy Materials*, **2020**, 10, 1902881	21.8	88
153	Hidden structural and chemical order controls lithium transport in cation-disordered oxides for rechargeable batteries. *Nature Communications*, **2019**, 10, 592	17.4	87

152	Constructing first-principles phase diagrams of amorphous LiSi using machine-learning-assisted sampling with an evolutionary algorithm. *Journal of Chemical Physics*, **2018**, 148, 241711	3.9	86
151	Computational and Experimental Investigations of Na-Ion Conduction in Cubic Na3PSe4. *Chemistry of Materials*, **2016**, 28, 252-258	9.6	83
150	Electronic-Structure Origin of Cation Disorder in Transition-Metal Oxides. *Physical Review Letters*, **2017**, 119, 176402	7.4	82
149	Design of Li1+2xZn1⊠PS4, a new lithium ion conductor. *Energy and Environmental Science*, **2016**, 9, 3272-3278	35.4	81
148	Design principles for high transition metal capacity in disordered rocksalt Li-ion cathodes. *Energy and Environmental Science*, **2018**, 11, 2159-2171	35.4	81
147	Reactivity-Guided Interface Design in Na Metal Solid-State Batteries. *Joule*, **2019**, 3, 1037-1050	27.8	80
146	Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. *Chemistry of Materials*, **2017**, 29, 6936-6946	9.6	78
145	Improved Cycling Performance of Li-Excess Cation-Disordered Cathode Materials upon Fluorine Substitution. *Advanced Energy Materials*, **2019**, 9, 1802959	21.8	77
144	Bayesian approach to cluster expansions. *Physical Review B*, **2009**, 80,	3.3	75
143	Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries. *Chemistry of Materials*, **2018**, 30, 6532-6539	9.6	73
142	Computational and experimental investigation of TmAgTe2 and XYZ2 compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening. *Journal of Materials Chemistry C*, **2015**, 3, 10554-10565	7.1	72
141	Fluorination of Lithium-Excess Transition Metal Oxide Cathode Materials. *Advanced Energy Materials*, **2018**, 8, 1701533	21.8	67
140	Ab initio investigation of the stability of electrolyte/electrode interfaces in all-solid-state Na batteries. *Journal of Materials Chemistry A*, **2019**, 7, 8144-8155	13	65
139	Understanding crystallization pathways leading to manganese oxide polymorph formation. *Nature Communications*, **2018**, 9, 2553	17.4	65
138	Vacancy Ordering in O3-Type Layered Metal Oxide Sodium-Ion Battery Cathodes. *Physical Review Applied*, **2015**, 4,	4.3	64
137	Phase diagram and electrochemical properties of mixed olivines from first-principles calculations. *Physical Review B*, **2009**, 79,	3.3	61
136	Size and charge effects on the structural stability of LiMO2 (M = transition metal) compounds. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1998**, 77, 1039-1047		61
135	Computational Design and Preparation of Cation-Disordered Oxides for High-Energy-Density Li-Ion Batteries. *Advanced Energy Materials*, **2016**, 6, 1600488	21.8	60

134	Structural and Na-ion conduction characteristics of Na3PSxSe4-x. *Journal of Materials Chemistry A*, **2016**, 4, 9044-9053	13	60
133	Ab initio study of the composition dependence of the pressure-induced spin transition in the (Mg1-x,Fex)O system. *Geophysical Research Letters*, **2006**, 33,	4.9	59
132	A Model to Compute Phase Diagrams in Oxides with Empirical or First-Principles Energy Methods and Application to the Solubility Limits in the CaO-MgO System. *Journal of the American Ceramic Society*, **1996**, 79, 2033-2040	3.8	59
131	Understanding the Effect of Cation Disorder on the Voltage Profile of Lithium Transition-Metal Oxides. *Chemistry of Materials*, **2016**, 28, 5373-5383	9.6	58
130	Structural and Compositional Factors That Control the Li-Ion Conductivity in LiPON Electrolytes. *Chemistry of Materials*, **2018**, 30, 7077-7090	9.6	58
129	Electrolyte-Induced Surface Transformation and Transition-Metal Dissolution of Fully Delithiated LiNiCoAlO. *Langmuir*, **2017**, 33, 9333-9353	4	57
128	The interplay between thermodynamics and kinetics in the solid-state synthesis of layered oxides. *Nature Materials*, **2020**, 19, 1088-1095	27	57
127	Influence of Inversion on Mg Mobility and Electrochemistry in Spinels. *Chemistry of Materials*, **2017**, 29, 7918-7930	9.6	55
126	Band structure engineering through orbital interaction for enhanced thermoelectric power factor. *Applied Physics Letters*, **2014**, 104, 082107	3.4	55
125	Explaining Performance-Limiting Mechanisms in Fluorophosphate Na-Ion Battery Cathodes through Inactive Transition-Metal Mixing and First-Principles Mobility Calculations. *Chemistry of Materials*, **2015**, 27, 6008-6015	9.6	54
124	Perspectives on Cobalt Supply through 2030 in the Face of Changing Demand. *Environmental Science & Technology*, **2020**, 54, 2985-2993	10.3	54
123	Design Principles for High-Capacity Mn-Based Cation-Disordered Rocksalt Cathodes. *CheM*, **2020**, 6, 153-168	16.8	54
122	First-Principles Simulation of the (LiNi-Vacancy)O Phase Diagram and Its Relevance for the Surface Phases in Ni-Rich Li-Ion Cathode Materials. *Chemistry of Materials*, **2017**, 29, 7840-7851	9.6	52
121	Synthesis and Electrochemical Properties of Layered Li0.9Ni0.45Ti0.55O2. *Chemistry of Materials*, **2003**, 15, 4503-4507	9.6	52
120	Deposition and Stripping Behavior of Lithium Metal in Electrochemical System: Continuum Mechanics Study. *Chemistry of Materials*, **2018**, 30, 6769-6776	9.6	52
119	Next-Generation Cathode Materials for Non-aqueous Potassium-Ion Batteries. *Trends in Chemistry*, **2019**, 1, 682-692	14.8	50
118	A High-Energy NASICON-Type Cathode Material for Na-Ion Batteries. *Advanced Energy Materials*, **2020**, 10, 1903968	21.8	50
117	Structure and Dynamics of Fluorophosphate Na-Ion Battery Cathodes. *Chemistry of Materials*, **2016**, 28, 5450-5460	9.6	49

116	Electrodeposition and Mechanical Stability at Lithium-Solid Electrolyte Interface during Plating in Solid-State Batteries. *Cell Reports Physical Science*, **2020**, 1, 100106	6.1	48
115	Text-mined dataset of inorganic materials synthesis recipes. *Scientific Data*, **2019**, 6, 203	8.2	48
114	Synthesis, Electrochemical Properties, and Phase Stability of Li2NiO2 with the Immm Structure. *Chemistry of Materials*, **2004**, 16, 2685-2690	9.6	48
113	Short-Range Order and Unusual Modes of Nickel Redox in a Fluorine-Substituted Disordered Rocksalt Oxide Lithium-Ion Cathode. *Chemistry of Materials*, **2018**, 30, 6945-6956	9.6	48
112	Band convergence in the non-cubic chalcopyrite compounds Cu2MGeSe4. *Journal of Materials Chemistry C*, **2014**, 2, 10189-10194	7.1	47
111	First principles study of Li diffusion in I-Li2NiO2 structure. *Physical Review B*, **2009**, 79,	3.3	47
110	Evaluating structure selection in the hydrothermal growth of FeS pyrite and marcasite. *Nature Communications*, **2016**, 7, 13799	17.4	47
109	Electrochemical properties and structural evolution of O3-type layered sodium mixed transition metal oxides with trivalent nickel. *Journal of Materials Chemistry A*, **2017**, 5, 4596-4606	13	46
108	NMR, PDF and RMC study of the positive electrode material Li(Ni0.5Mn0.5)O2 synthesized by ion-exchange methods. *Journal of Materials Chemistry*, **2007**, 17, 3167		45
107	Designing new lithium-excess cathode materials from percolation theory: nanohighways in Li(x)Ni(2-4x/3)Sb(x/3)O2. *Nano Letters*, **2015**, 15, 596-602	11.5	44
106	Localized concentration reversal of lithium during intercalation into nanoparticles. *Science Advances*, **2018**, 4, eaao2608	14.3	44
105	The Effect of Cation Disorder on the Average Li Intercalation Voltage of Transition-Metal Oxides. *Chemistry of Materials*, **2016**, 28, 3659-3665	9.6	44
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	13	43
103	Computational Prediction and Evaluation of Solid-State Sodium Superionic Conductors Na7P3X11 (X = O, S, Se). *Chemistry of Materials*, **2017**, 29, 7475-7482	9.6	43
102	A critical examination of compound stability predictions from machine-learned formation energies. *Npj Computational Materials*, **2020**, 6,	10.9	42
101	Semi-supervised machine-learning classification of materials synthesis procedures. *Npj Computational Materials*, **2019**, 5,	10.9	39
100	Particle-size and morphology dependence of the preferred interface orientation in LiFePO4 nano-particles. *Journal of Materials Chemistry A*, **2014**, 2, 15437-15447	13	37
99	Characterization of mechanical degradation in an all-solid-state battery cathode. *Journal of Materials Chemistry A*, **2020**, 8, 17399-17404	13	37

98	First-Principles Study of the Voltage Profile and Mobility of Mg Intercalation in a Chromium Oxide Spinel. *Chemistry of Materials*, **2018**, 30, 153-162	9.6	37
97	Understanding Surface Densified Phases in Ni-Rich Layered Compounds. *ACS Energy Letters*, **2019**, 4, 811-818	20.1	36
96	Data-driven materials research enabled by natural language processing and information extraction. *Applied Physics Reviews*, **2020**, 7, 041317	17.3	36
95	Direct Visualization of the Interfacial Degradation of Cathode Coatings in Solid State Batteries: A Combined Experimental and Computational Study. *Advanced Energy Materials*, **2020**, 10, 1903778	21.8	36
94	Electrochemically controlled transport of lithium through ultrathin SiO2. *Journal of Applied Physics*, **2005**, 98, 023516	2.5	36
93	Architecture Dependence on the Dynamics of Nano-LiFePO4 Electrodes. *Electrochimica Acta*, **2014**, 137, 245-257	6.7	35
92	High-fraction brookite films from amorphous precursors. *Scientific Reports*, **2017**, 7, 15232	4.9	35
91	Effect of Fluorination on Lithium Transport and Short-Range Order in Disordered-Rocksalt-Type Lithium-Ion Battery Cathodes. *Advanced Energy Materials*, **2020**, 10, 1903240	21.8	34
90	Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. *Journal of the American Chemical Society*, **2018**, 140, 4293-4301	16.4	34
89	Ion-exchange mechanism of layered transition-metal oxides: case study of LiNi(0.5)Mn(0.5)O□ *Inorganic Chemistry*, **2014**, 53, 8083-7	5.1	34
88	Synthesis and electrochemical properties of layered LiNi2/3Sb1/3O2. *Journal of Power Sources*, **2007**, 173, 550-555	8.9	34
87	Non-equilibrium crystallization pathways of manganese oxides in aqueous solution. *Nature Communications*, **2019**, 10, 573	17.4	33
86	Induction time of a polymorphic transformation. *CrystEngComm*, **2017**, 19, 4576-4585	3.3	32
85	An efficient algorithm for finding the minimum energy path for cation migration in ionic materials. *Journal of Chemical Physics*, **2016**, 145, 074112	3.9	32
84	Predictive modeling and design rules for solid electrolytes. *MRS Bulletin*, **2018**, 43, 746-751	3.2	31
83	Computational Investigation and Experimental Realization of Disordered High-Capacity Li-Ion Cathodes Based on Ni Redox. *Chemistry of Materials*, **2019**, 31, 2431-2442	9.6	30
82	On the Balance of Intercalation and Conversion Reactions in Battery Cathodes. *Advanced Energy Materials*, **2018**, 8, 1800379	21.8	30
81	Evaluation of Mg Compounds as Coating Materials in Mg Batteries. *Frontiers in Chemistry*, **2019**, 7, 24	5	27

80	Theoretical capacity achieved in a LiMn0.5Fe0.4Mg0.1BO3 cathode by using topological disorder. *Energy and Environmental Science*, **2015**, 8, 1790-1798	35.4	27
79	An Analysis of Solid-State Electrodeposition-Induced Metal Plastic Flow and Predictions of Stress States in Solid Ionic Conductor Defects. *Journal of the Electrochemical Society*, **2020**, 167, 020534	3.9	27
78	Rationalizing accurate structure prediction in the meta-GGA SCAN functional. *Physical Review B*, **2019**, 100,	3.3	27
77	Data-mined similarity function between material compositions. *Physical Review B*, **2013**, 88,	3.3	26
76	Thermodynamics of Oxides with Substitutional Disorder: A Microscopic Model and Evaluation of Important Energy Contributions. *Journal of the American Ceramic Society*, **2005**, 81, 517-525	3.8	26
75	Probing Mg Migration in Spinel Oxides. *Chemistry of Materials*, **2020**, 32, 663-670	9.6	26
74	A First-Principles and Experimental Investigation of Nickel Solubility into the P2 NaxCoO2 Sodium-Ion Cathode. *Advanced Energy Materials*, **2018**, 8, 1801446	21.8	25
73	Synthesis and Electrochemical Properties of I4 -Type Li1+2xZn1⊠PS4 Solid Electrolyte. *Chemistry of Materials*, **2018**, 30, 2236-2244	9.6	24
72	Revealing and Rationalizing the Rich Polytypism of Todorokite MnO. *Journal of the American Chemical Society*, **2018**, 140, 6961-6968	16.4	24
71	Effect of a Size-Dependent Equilibrium Potential on Nano-LiFePO4Particle Interactions. *Journal of the Electrochemical Society*, **2015**, 162, A1718-A1724	3.9	24
70	The Effect of Antisite Disorder and Particle Size on Li Intercalation Kinetics in Monoclinic LiMnBO3. *Advanced Energy Materials*, **2015**, 5, 1401916	21.8	24
69	Kinetics of Nanoparticle Interactions in Battery Electrodes. *Journal of the Electrochemical Society*, **2015**, 162, A965-A973	3.9	23
68	Analysis of Charged State Stability for Monoclinic LiMnBO3 Cathode. *Chemistry of Materials*, **2014**, 26, 4200-4206	9.6	23
67	Li-ion conductivity in Li9S3N. *Journal of Materials Chemistry A*, **2015**, 3, 20338-20344	13	22
66	Impact of intermediate sites on bulk diffusion barriers: Mg intercalation in Mg2Mo3O8. *Journal of Materials Chemistry A*, **2016**, 4, 17643-17648	13	22
65	Magnesium ion mobility in post-spinels accessible at ambient pressure. *Chemical Communications*, **2017**, 53, 5171-5174	5.8	19
64	Investigation of Alkali-Ion (Li, Na, and K) Intercalation in KxVPO4F (x ~ 0) Cathode. *Advanced Functional Materials*, **2019**, 29, 1902392	15.6	19
63	Fast Mg diffusion in Mo(PO)O for Mg batteries. *Chemical Communications*, **2017**, 53, 7998-8001	5.8	19

62	Distilling a Materials Synthesis Ontology. *Matter*, **2019**, 1, 8-12	12.7	18
61	Finding and proving the exact ground state of a generalized Ising model by convex optimization and MAX-SAT. *Physical Review B*, **2016**, 94,	3.3	18
60	Opportunities and challenges of text mining in aterials research. *IScience*, **2021**, 24, 102155	6.1	18
59	Direct Observation of Alternating Octahedral and Prismatic Sodium Layers in O3-Type Transition Metal Oxides. *Advanced Energy Materials*, **2020**, 10, 2001151	21.8	16
58	Toward autonomous design and synthesis of novel inorganic materials. *Materials Horizons*, **2021**, 8, 2169-2198	14.4	16
57	Observing and Modeling the Sequential Pairwise Reactions that Drive Solid-State Ceramic Synthesis. *Advanced Materials*, **2021**, 33, e2100312	24	14
56	Zn2SbN3: growth and characterization of a metastable photoactive semiconductor. *Materials Horizons*, **2019**, 6, 1669-1674	14.4	13
55	Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite-Size Ion Models. *Journal of Physical Chemistry Letters*, **2018**, 9, 628-634	6.4	13
54	First Principles Study on Ta3N5:Ti3O3N2Solid Solution As a Water-Splitting Photocatalyst. *Journal of Physical Chemistry C*, **2013**, 117, 24710-24715	3.8	13
53	Similarity of Precursors in Solid-State Synthesis as Text-Mined from Scientific Literature. *Chemistry of Materials*, **2020**, 32, 7861-7873	9.6	13
52	A bio-facilitated synthetic route for nano-structured complex electrode materials. *Green Chemistry*, **2016**, 18, 2619-2624	10	13
51	Probabilistic Deep Learning Approach to Automate the Interpretation of Multi-phase Diffraction Spectra. *Chemistry of Materials*, **2021**, 33, 4204-4215	9.6	12
50	Shear-Assisted Formation of Cation-Disordered Rocksalt NaMO2 (M = Fe or Mn). *Chemistry of Materials*, **2018**, 30, 8811-8821	9.6	12
49	Lithium superionic conductors with corner-sharing frameworks.. *Nature Materials*, **2022**,	27	12
48	Communication□O3-Type Layered Oxide with a Quaternary Transition Metal Composition for Na-Ion Battery Cathodes: NaTi0.25Fe0.25Co0.25Ni0.25O2. *Journal of the Electrochemical Society*, **2017**, 164, A3484-A3486	3.9	11
47	Manufacturing scalability implications of materials choice in inorganic solid-state batteries. *Joule*, **2021**, 5, 564-580	27.8	11
46	Fluorination-Enhanced Surface Stability of Cation-Disordered Rocksalt Cathodes for Li-Ion Batteries. *Advanced Functional Materials*, **2021**, 31, 2101888	15.6	11
45	Selective metathesis synthesis of MgCr2S4 by control of thermodynamic driving forces. *Materials Horizons*, **2020**, 7, 1310-1316	14.4	10

44	Na+ Redistribution by Electrochemical Na+/K+ Exchange in Layered NaxNi2SbO6. *Chemistry of Materials*, **2020**, 32, 4312-4323	9.6	10
43	Non-topotactic reactions enable high rate capability in Li-rich cathode materials. *Nature Energy*,	62.3	10
42	Computational investigation of dielectric absorption at microwave frequencies in binary oxides. *Journal of Applied Physics*, **2001**, 89, 5630-5636	2.5	9
41	The Impact of Surface Structure Transformations on the Performance of Li-Excess Cation-Disordered Rocksalt Cathodes. *Cell Reports Physical Science*, **2020**, 1, 100187	6.1	8
40	Construction of ground-state preserving sparse lattice models for predictive materials simulations. *Npj Computational Materials*, **2017**, 3,	10.9	8
39	Earth abundant materials for high efficiency heterojunction thin film solar cells **2009**,		8
38	Origin of Capacity Degradation of High-Voltage KVPO4F Cathode. *Journal of the Electrochemical Society*, **2020**, 167, 110555	3.9	8
37	Kinetic Pathways Templated by Low-Temperature Intermediates during Solid-State Synthesis of Layered Oxides. *Chemistry of Materials*, **2020**, 32, 9906-9913	9.6	8
36	Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials. *Journal of Materials Chemistry A*, **2020**, 8, 19965-19974	13	8
35	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	9.6	7
34	Atomic Structure of Surface-Densified Phases in Ni-Rich Layered Compounds. *ACS Applied Materials & Interfaces*, **2021**, 13, 17478-17486	9.5	7
33	Lithium Oxide Superionic Conductors Inspired by Garnet and NASICON Structures. *Advanced Energy Materials*, **2021**, 11, 2101437	21.8	7
32	Synthetic accessibility and stability rules of NASICONs. *Nature Communications*, **2021**, 12, 5752	17.4	7
31	The effect of surface-bulk potential difference on the kinetics of intercalation in core-shell active cathode particles. *Journal of Power Sources*, **2018**, 382, 30-37	8.9	6
30	Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes. *Matter*, **2021**,	12.7	6
29	Increasing Capacity in Disordered Rocksalt Cathodes by Mg Doping. *Chemistry of Materials*, **2020**, 32, 10728-10736	9.6	6
28	Ab INITIO CALCULATION OF THE LixCoO2 PHASE DIAGRAM. *Materials Research Society Symposia Proceedings*, **1997**, 496, 121		5
27	First-principles estimate of the order□disorder transition in Ba(ZnxNb1□)O3 microwave dielectrics. *Journal of Materials Research*, **2000**, 15, 2061-2064	2.5	5

26	All-Solid-State Batteries: High Active Material Loading in All-Solid-State Battery Electrode via Particle Size Optimization (Adv. Energy Mater. 1/2020). *Advanced Energy Materials*, **2020**, 10, 2070004	21.8	5
25	First-principles study of CaBH as a potential solid-state conductor for Ca. *Physical Chemistry Chemical Physics*, **2020**, 22, 27600-27604	3.6	5
24	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	16.4	5
23	Computational Investigation of Halogen-Substituted Na Argyrodites as Solid-State Superionic Conductors. *Chemistry of Materials*, **2020**, 32, 1896-1903	9.6	4
22	Computational and experimental search for potential polyanionic K-ion cathode materials. *Journal of Materials Chemistry A*, **2021**, 9, 18564-18575	13	4
21	Electrodes: The Configurational Space of Rocksalt-Type Oxides for High-Capacity Lithium Battery Electrodes (Adv. Energy Mater. 13/2014). *Advanced Energy Materials*, **2014**, 4, n/a-n/a	21.8	3
20	A Drastic Influence of Point Defects on Phase Stability in MnO2. *Materials Research Society Symposia Proceedings*, **2002**, 755, 1		3
19	Insights into Layered Oxide Cathodes for Rechargeable Batteries. *Molecules*, **2021**, 26,	4.8	3
18	Data Mining Approach to Ab-Initio Prediction of Crystal Structure. *Materials Research Society Symposia Proceedings*, **2003**, 804, 305		2
17	Ground State Analysis on the FCC Lattice with Four Pair Interactions. *Materials Research Society Symposia Proceedings*, **1992**, 291, 259		2
16	Toward the Development of a High-Voltage Mg Cathode Using a Chromium Sulfide Host **2021**, 3, 1213-1220		2
15	Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science.. *Patterns*, **2022**, 3, 100488	5.1	2
14	Thermodynamically Driven Synthetic Optimization for Cation-Disordered Rock Salt Cathodes. *Advanced Energy Materials*,2103923	21.8	2
13	Phase Transformations in Hexagonal-Close-Packed Alloys: Analysis with the Cluster Variation Method. *Materials Research Society Symposia Proceedings*, **1992**, 291, 395		1
12	Understanding the Formation Energy of Transition Metal Hydrides. *Materials Research Society Symposia Proceedings*, **2002**, 730, 1		1
11	Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic First-Principles Evaluation. *Advanced Energy Materials*,2101698	21.8	1
10	Understanding Crystallization Pathways of MnOx Polymorph Formation via in-situ X-ray Scattering. *Microscopy and Microanalysis*, **2018**, 24, 1486-1487	0.5	1
9	Online Interactive Platform for COVID-19 Literature Visual Analytics: Platform Development Study. *Journal of Medical Internet Research*, **2021**, 23, e26995	7.6	1

8	Expanding the Ambient-Pressure Phase Space of CaFe2O4-Type Sodium Postspinel Host⊡Guest Compounds. *ACS Organic & Inorganic Au*,		1
7	Solid-State Calcium-Ion Diffusion in Ca1.5Ba0.5Si5O3N6. *Chemistry of Materials*, **2022**, 34, 128-139	9.6	1
6	Intercalation of Ca into a Highly Defective Manganese Oxide at Room Temperature. *Chemistry of Materials*, **2022**, 34, 836-846	9.6	0
5	Dynamic Barriers to Crystallization of Calcium Barium Carbonates. *Crystal Growth and Design*, **2021**, 21, 4556-4563	3.5	0
4	Kinetic origins of the metastable zone width in the manganese oxide Pourbaix diagram. *Journal of Materials Chemistry A*, **2021**, 9, 7857-7867	13	0
3	Dynamics and Thermodynamics of a system with multiple length scales. *Materials Research Society Symposia Proceedings*, **2002**, 731, 441		
2	Oxygen Configurations and their Effect on Charge Transfer in YBa2Cu3OZ. *Materials Research Society Symposia Proceedings*, **1992**, 278, 103		
1	The Interplay between Thermodynamics and Kinetics in the Solid-State Synthesis of Layered Oxides. *ECS Meeting Abstracts*, **2020**, MA2020-02, 313-313	0	