Gerbrand Ceder

List of Publications by Citations

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	33.3	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	LiFePO4 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, 656-63	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	Jahn□eller 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−xPS4, 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	19.1	54
122	First-Principles Simulation of the (LiNiVacancy)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	