# Gerbrand Ceder

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | Intercalation of Ca into a Highly Defective Manganese Oxide at Room Temperature. *Chemistry of Materials*, **2022**, 34, 836-846 | 9.6 | 0 |
| 258 | Lithium superionic conductors with corner-sharing frameworks.. *Nature Materials*, **2022**, | 27 | 12 |
| 257 | Quantifying the advantage of domain-specific pre-training on named entity recognition tasks in materials science.. *Patterns*, **2022**, 3, 100488 | 5.1 | 2 |
| 256 | Solid-State Calcium-Ion Diffusion in Ca1.5Ba0.5Si5O3N6. *Chemistry of Materials*, **2022**, 34, 128-139 | 9.6 | 1 |
| 255 | Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes. *Matter*, **2021**, | 12.7 | 6 |
| 254 | Manufacturing scalability implications of materials choice in inorganic solid-state batteries. *Joule*, **2021**, 5, 564-580 | 27.8 | 11 |
| 253 | Fluorination-Enhanced Surface Stability of Cation-Disordered Rocksalt Cathodes for Li-Ion Batteries. *Advanced Functional Materials*, **2021**, 31, 2101888 | 15.6 | 11 |
| 252 | Atomic Structure of Surface-Densified Phases in Ni-Rich Layered Compounds. *ACS Applied Materials & Interfaces*, **2021**, 13, 17478-17486 | 9.5 | 7 |
| 251 | Insights into Layered Oxide Cathodes for Rechargeable Batteries. *Molecules*, **2021**, 26, | 4.8 | 3 |
| 250 | Observing and Modeling the Sequential Pairwise Reactions that Drive Solid-State Ceramic Synthesis. *Advanced Materials*, **2021**, 33, e2100312 | 24 | 14 |
| 249 | Probabilistic Deep Learning Approach to Automate the Interpretation of Multi-phase Diffraction Spectra. *Chemistry of Materials*, **2021**, 33, 4204-4215 | 9.6 | 12 |
| 248 | Dynamic Barriers to Crystallization of Calcium Barium Carbonates. *Crystal Growth and Design*, **2021**, 21, 4556-4563 | 3.5 | 0 |
| 247 | 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 |
| 246 | Cation-disordered rocksalt-type high-entropy cathodes for Li-ion batteries. *Nature Materials*, **2021**, 20, 214-221 | 27 | 90 |
| 245 | 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 |
| 244 | Computational and experimental search for potential polyanionic K-ion cathode materials. *Journal of Materials Chemistry A*, **2021**, 9, 18564-18575 | 13 | 4 |
| 243 | Toward autonomous design and synthesis of novel inorganic materials. *Materials Horizons*, **2021**, 8, 2169-2198 | 14.4 | 16 |

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| 242 | Opportunities and challenges of text mining in aterials research. *IScience*, **2021**, 24, 102155 | 6.1 | 18 |
| 241 | Toward the Development of a High-Voltage Mg Cathode Using a Chromium Sulfide Host **2021**, 3, 1213-1220 | | 2 |
| 240 | Online Interactive Platform for COVID-19 Literature Visual Analytics: Platform Development Study. *Journal of Medical Internet Research*, **2021**, 23, e26995 | 7.6 | 1 |
| 239 | Lithium Oxide Superionic Conductors Inspired by Garnet and NASICON Structures. *Advanced Energy Materials*, **2021**, 11, 2101437 | 21.8 | 7 |
| 238 | Synthetic accessibility and stability rules of NASICONs. *Nature Communications*, **2021**, 12, 5752 | 17.4 | 7 |
| 237 | Kinetic origins of the metastable zone width in the manganese oxide Pourbaix diagram. *Journal of Materials Chemistry A*, **2021**, 9, 7857-7867 | 13 | 0 |
| 236 | Data-driven materials research enabled by natural language processing and information extraction. *Applied Physics Reviews*, **2020**, 7, 041317 | 17.3 | 36 |
| 235 | 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 |
| 234 | The interplay between thermodynamics and kinetics in the solid-state synthesis of layered oxides. *Nature Materials*, **2020**, 19, 1088-1095 | 27 | 57 |
| 233 | 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 |
| 232 | 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 |
| 231 | Ultrahigh power and energy density in partially ordered lithium-ion cathode materials. *Nature Energy*, **2020**, 5, 213-221 | 62.3 | 91 |
| 230 | Direct Observation of Alternating Octahedral and Prismatic Sodium Layers in O3-Type Transition Metal Oxides. *Advanced Energy Materials*, **2020**, 10, 2001151 | 21.8 | 16 |
| 229 | 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 |
| 228 | 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 |
| 227 | Kinetic pathways of ionic transport in fast-charging lithium titanate. *Science*, **2020**, 367, 1030-1034 | 33.3 | 95 |
| 226 | Perspectives on Cobalt Supply through 2030 in the Face of Changing Demand. *Environmental Science & Technology*, **2020**, 54, 2985-2993 | 10.3 | 54 |
| 225 | Selective metathesis synthesis of MgCr2S4 by control of thermodynamic driving forces. *Materials Horizons*, **2020**, 7, 1310-1316 | 14.4 | 10 |

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| 224 | Computational Investigation of Halogen-Substituted Na Argyrodites as Solid-State Superionic Conductors. *Chemistry of Materials*, **2020**, 32, 1896-1903 | 9.6 | 4 |
| 223 | 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 |
| 222 | Na+ Redistribution by Electrochemical Na+/K+ Exchange in Layered NaxNi2SbO6. *Chemistry of Materials*, **2020**, 32, 4312-4323 | 9.6 | 10 |
| 221 | The Interplay between Thermodynamics and Kinetics in the Solid-State Synthesis of Layered Oxides. *ECS Meeting Abstracts*, **2020**, MA2020-02, 313-313 | 0 | |
| 220 | Origin of Capacity Degradation of High-Voltage KVPO4F Cathode. *Journal of the Electrochemical Society*, **2020**, 167, 110555 | 3.9 | 8 |
| 219 | 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 |
| 218 | Probing Mg Migration in Spinel Oxides. *Chemistry of Materials*, **2020**, 32, 663-670 | 9.6 | 26 |
| 217 | Understanding interface stability in solid-state batteries. *Nature Reviews Materials*, **2020**, 5, 105-126 | 73.3 | 318 |
| 216 | High Active Material Loading in All-Solid-State Battery Electrode via Particle Size Optimization. *Advanced Energy Materials*, **2020**, 10, 1902881 | 21.8 | 88 |
| 215 | 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 |
| 214 | Increasing Capacity in Disordered Rocksalt Cathodes by Mg Doping. *Chemistry of Materials*, **2020**, 32, 10728-10736 | 9.6 | 6 |
| 213 | First-principles study of CaBH as a potential solid-state conductor for Ca. *Physical Chemistry Chemical Physics*, **2020**, 22, 27600-27604 | 3.6 | 5 |
| 212 | Kinetic Pathways Templated by Low-Temperature Intermediates during Solid-State Synthesis of Layered Oxides. *Chemistry of Materials*, **2020**, 32, 9906-9913 | 9.6 | 8 |
| 211 | 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 |
| 210 | Similarity of Precursors in Solid-State Synthesis as Text-Mined from Scientific Literature. *Chemistry of Materials*, **2020**, 32, 7861-7873 | 9.6 | 13 |
| 209 | Characterization of mechanical degradation in an all-solid-state battery cathode. *Journal of Materials Chemistry A*, **2020**, 8, 17399-17404 | 13 | 37 |
| 208 | A critical examination of compound stability predictions from machine-learned formation energies. *Npj Computational Materials*, **2020**, 6, | 10.9 | 42 |
| 207 | Design Principles for High-Capacity Mn-Based Cation-Disordered Rocksalt Cathodes. *CheM*, **2020**, 6, 153-168 | 18 | 54 |

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| 206 | A High-Energy NASICON-Type Cathode Material for Na-Ion Batteries. *Advanced Energy Materials*, **2020**, 10, 1903968 | 21.8 | 50 |
| 205 | Reactivity-Guided Interface Design in Na Metal Solid-State Batteries. *Joule*, **2019**, 3, 1037-1050 | 27.8 | 80 |
| 204 | Metal-oxygen decoordination stabilizes anion redox in Li-rich oxides. *Nature Materials*, **2019**, 18, 256-265 | 27 | 178 |
| 203 | A map of the inorganic ternary metal nitrides. *Nature Materials*, **2019**, 18, 732-739 | 27 | 148 |
| 202 | Investigation of Alkali-Ion (Li, Na, and K) Intercalation in KxVPO4F (x ~ 0) Cathode. *Advanced Functional Materials*, **2019**, 29, 1902392 | 15.6 | 19 |
| 201 | Distilling a Materials Synthesis Ontology. *Matter*, **2019**, 1, 8-12 | 12.7 | 18 |
| 200 | Next-Generation Cathode Materials for Non-aqueous Potassium-Ion Batteries. *Trends in Chemistry*, **2019**, 1, 682-692 | 14.8 | 50 |
| 199 | Zn2SbN3: growth and characterization of a metastable photoactive semiconductor. *Materials Horizons*, **2019**, 6, 1669-1674 | 14.4 | 13 |
| 198 | Computational Screening of Cathode Coatings for Solid-State Batteries. *Joule*, **2019**, 3, 1252-1275 | 27.8 | 162 |
| 197 | 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 |
| 196 | Hidden structural and chemical order controls lithium transport in cation-disordered oxides for rechargeable batteries. *Nature Communications*, **2019**, 10, 592 | 17.4 | 87 |
| 195 | Evaluation of Mg Compounds as Coating Materials in Mg Batteries. *Frontiers in Chemistry*, **2019**, 7, 24 | 5 | 27 |
| 194 | Non-equilibrium crystallization pathways of manganese oxides in aqueous solution. *Nature Communications*, **2019**, 10, 573 | 17.4 | 33 |
| 193 | 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 |
| 192 | Understanding Surface Densified Phases in Ni-Rich Layered Compounds. *ACS Energy Letters*, **2019**, 4, 811-818 | 20.1 | 36 |
| 191 | Rationalizing accurate structure prediction in the meta-GGA SCAN functional. *Physical Review B*, **2019**, 100, | 3.3 | 27 |
| 190 | Semi-supervised machine-learning classification of materials synthesis procedures. *Npj Computational Materials*, **2019**, 5, | 10.9 | 39 |
| 189 | Unsupervised word embeddings capture latent knowledge from materials science literature. *Nature*, **2019**, 571, 95-98 | 50.4 | 325 |

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| 188 | Text-mined dataset of inorganic materials synthesis recipes. *Scientific Data*, **2019**, 6, 203 | 8.2 | 48 |
| 187 | Improved Cycling Performance of Li-Excess Cation-Disordered Cathode Materials upon Fluorine Substitution. *Advanced Energy Materials*, **2019**, 9, 1802959 | 21.8 | 77 |
| 186 | Synthesis and Electrochemical Properties of I4 -Type Li1+2xZn1−xPS4 Solid Electrolyte. *Chemistry of Materials*, **2018**, 30, 2236-2244 | 9.6 | 24 |
| 185 | Redox-Mediated Stabilization in Zinc Molybdenum Nitrides. *Journal of the American Chemical Society*, **2018**, 140, 4293-4301 | 16.4 | 34 |
| 184 | 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 |
| 183 | On the Balance of Intercalation and Conversion Reactions in Battery Cathodes. *Advanced Energy Materials*, **2018**, 8, 1800379 | 21.8 | 30 |
| 182 | Reversible Mn/Mn double redox in lithium-excess cathode materials. *Nature*, **2018**, 556, 185-190 | 50.4 | 376 |
| 181 | Localized concentration reversal of lithium during intercalation into nanoparticles. *Science Advances*, **2018**, 4, eaao2608 | 14.3 | 44 |
| 180 | Electrostatic Estimation of Intercalant Jump-Diffusion Barriers Using Finite-Size Ion Models. *Journal of Physical Chemistry Letters*, **2018**, 9, 628-634 | 6.4 | 13 |
| 179 | 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 |
| 178 | Efficient first-principles prediction of solid stability: Towards chemical accuracy. *Npj Computational Materials*, **2018**, 4, | 10.9 | 107 |
| 177 | Fluorination of Lithium-Excess Transition Metal Oxide Cathode Materials. *Advanced Energy Materials*, **2018**, 8, 1701533 | 21.8 | 67 |
| 176 | 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 |
| 175 | A New Strategy for High-Voltage Cathodes for K-Ion Batteries: Stoichiometric KVPO4F. *Advanced Energy Materials*, **2018**, 8, 1801591 | 21.8 | 90 |
| 174 | Revealing and Rationalizing the Rich Polytypism of Todorokite MnO. *Journal of the American Chemical Society*, **2018**, 140, 6961-6968 | 16.4 | 24 |
| 173 | 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 |
| 172 | Recent Progress and Perspective in Electrode Materials for K-Ion Batteries. *Advanced Energy Materials*, **2018**, 8, 1702384 | 21.8 | 428 |
| 171 | Shear-Assisted Formation of Cation-Disordered Rocksalt NaMO2 (M = Fe or Mn). *Chemistry of Materials*, **2018**, 30, 8811-8821 | 9.6 | 12 |

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| 170 | Understanding Crystallization Pathways of MnOx Polymorph Formation via in-situ X-ray Scattering. *Microscopy and Microanalysis*, **2018**, 24, 1486-1487 | 0.5 | 1 |
| 169 | Predictive modeling and design rules for solid electrolytes. *MRS Bulletin*, **2018**, 43, 746-751 | 3.2 | 31 |
| 168 | Structural and Compositional Factors That Control the Li-Ion Conductivity in LiPON Electrolytes. *Chemistry of Materials*, **2018**, 30, 7077-7090 | 9.6 | 58 |
| 167 | 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 |
| 166 | Deposition and Stripping Behavior of Lithium Metal in Electrochemical System: Continuum Mechanics Study. *Chemistry of Materials*, **2018**, 30, 6769-6776 | 9.6 | 52 |
| 165 | Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries. *Chemistry of Materials*, **2018**, 30, 6532-6539 | 9.6 | 73 |
| 164 | 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 |
| 163 | Design principles for high transition metal capacity in disordered rocksalt Li-ion cathodes. *Energy and Environmental Science*, **2018**, 11, 2159-2171 | 35.4 | 81 |
| 162 | Understanding crystallization pathways leading to manganese oxide polymorph formation. *Nature Communications*, **2018**, 9, 2553 | 17.4 | 65 |
| 161 | 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 |
| 160 | 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 |
| 159 | Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. *Chemical Reviews*, **2017**, 117, 4287-4341 | 68.1 | 687 |
| 158 | Magnesium ion mobility in post-spinels accessible at ambient pressure. *Chemical Communications*, **2017**, 53, 5171-5174 | 5.8 | 19 |
| 157 | Additional Sodium Insertion into Polyanionic Cathodes for Higher-Energy Na-Ion Batteries. *Advanced Energy Materials*, **2017**, 7, 1700514 | 21.8 | 116 |
| 156 | K-Ion Batteries Based on a P2-Type K0.6CoO2 Cathode. *Advanced Energy Materials*, **2017**, 7, 1700098 | 21.8 | 208 |
| 155 | Compatibility issues between electrodes and electrolytes in solid-state batteries. *Energy and Environmental Science*, **2017**, 10, 1150-1166 | 35.4 | 196 |
| 154 | Electrolyte-Induced Surface Transformation and Transition-Metal Dissolution of Fully Delithiated LiNiCoAlO. *Langmuir*, **2017**, 33, 9333-9353 | 4 | 57 |
| 153 | Effective mass and Fermi surface complexity factor from ab initio band structure calculations. *Npj Computational Materials*, **2017**, 3, | 10.9 | 92 |

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| 152 | Electronic-Structure Origin of Cation Disorder in Transition-Metal Oxides. *Physical Review Letters*, **2017**, 119, 176402 | 7.4 | 82 |
| 151 | Lithium-Ion Battery Supply Chain Considerations: Analysis of Potential Bottlenecks in Critical Metals. *Joule*, **2017**, 1, 229-243 | 27.8 | 581 |
| 150 | Mitigating oxygen loss to improve the cycling performance of high capacity cation-disordered cathode materials. *Nature Communications*, **2017**, 8, 981 | 17.4 | 136 |
| 149 | Materials Synthesis Insights from Scientific Literature via Text Extraction and Machine Learning. *Chemistry of Materials*, **2017**, 29, 9436-9444 | 9.6 | 202 |
| 148 | High magnesium mobility in ternary spinel chalcogenides. *Nature Communications*, **2017**, 8, 1759 | 17.4 | 137 |
| 147 | Influence of Inversion on Mg Mobility and Electrochemistry in Spinels. *Chemistry of Materials*, **2017**, 29, 7918-7930 | 9.6 | 55 |
| 146 | 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 |
| 145 | Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species. *Physical Review B*, **2017**, 96, | 3.3 | 163 |
| 144 | Induction time of a polymorphic transformation. *CrystEngComm*, **2017**, 19, 4576-4585 | 3.3 | 32 |
| 143 | Thermodynamic Routes to Novel Metastable Nitrogen-Rich Nitrides. *Chemistry of Materials*, **2017**, 29, 6936-6946 | 9.6 | 78 |
| 142 | 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 |
| 141 | Investigation of Potassium Storage in Layered P3-Type K MnO Cathode. *Advanced Materials*, **2017**, 29, 1702480 | 24 | 197 |
| 140 | Construction of ground-state preserving sparse lattice models for predictive materials simulations. *Npj Computational Materials*, **2017**, 3, | 10.9 | 8 |
| 139 | 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 |
| 138 | High-fraction brookite films from amorphous precursors. *Scientific Reports*, **2017**, 7, 15232 | 4.9 | 35 |
| 137 | Fast Mg diffusion in Mo(PO)O for Mg batteries. *Chemical Communications*, **2017**, 53, 7998-8001 | 5.8 | 19 |
| 136 | Jahn□Teller Assisted Na Diffusion for High Performance Na Ion Batteries. *Chemistry of Materials*, **2016**, 28, 6575-6583 | 9.6 | 89 |
| 135 | Evaluation of sulfur spinel compounds for multivalent battery cathode applications. *Energy and Environmental Science*, **2016**, 9, 3201-3209 | 35.4 | 91 |

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| 134 | Interface Stability in Solid-State Batteries. *Chemistry of Materials*, **2016**, 28, 266-273 | 9.6 | 792 |
| 133 | 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 |
| 132 | Design of Li1+2xZn1−xPS4, a new lithium ion conductor. *Energy and Environmental Science*, **2016**, 9, 3272-3278 | 33.4 | 81 |
| 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 | Energetics of MnO2 polymorphs in density functional theory. *Physical Review B*, **2016**, 93, | 3.3 | 147 |
| 129 | Structure and Dynamics of Fluorophosphate Na-Ion Battery Cathodes. *Chemistry of Materials*, **2016**, 28, 5450-5460 | 9.6 | 49 |
| 128 | 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 |
| 127 | The thermodynamic scale of inorganic crystalline metastability. *Science Advances*, **2016**, 2, e1600225 | 14.3 | 352 |
| 126 | Design and synthesis of the superionic conductor Na10SnP2S12. *Nature Communications*, **2016**, 7, 11009 | 17.4 | 193 |
| 125 | Impact of intermediate sites on bulk diffusion barriers: Mg intercalation in Mg2Mo3O8. *Journal of Materials Chemistry A*, **2016**, 4, 17643-17648 | 13 | 22 |
| 124 | Computational understanding of Li-ion batteries. *Npj Computational Materials*, **2016**, 2, | 10.9 | 299 |
| 123 | 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 |
| 122 | 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 |
| 121 | Role of Structural H2O in Intercalation Electrodes: The Case of Mg in Nanocrystalline Xerogel-V2O5. *Nano Letters*, **2016**, 16, 2426-31 | 11.5 | 146 |
| 120 | Layered-to-Rock-Salt Transformation in Desodiated NaxCrO2 (x 0.4). *Chemistry of Materials*, **2016**, 28, 1419-1429 | 9.6 | 100 |
| 119 | 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 |
| 118 | Computational and Experimental Investigations of Na-Ion Conduction in Cubic Na3PSe4. *Chemistry of Materials*, **2016**, 28, 252-258 | 9.6 | 83 |
| 117 | Computational Design and Preparation of Cation-Disordered Oxides for High-Energy-Density Li-Ion Batteries. *Advanced Energy Materials*, **2016**, 6, 1600488 | 21.8 | 60 |

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| 116 | Evaluating structure selection in the hydrothermal growth of FeS pyrite and marcasite. *Nature Communications*, **2016**, 7, 13799 | 17.4 | 47 |
| 115 | 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 |
| 114 | A high capacity thiospinel cathode for Mg batteries. *Energy and Environmental Science*, **2016**, 9, 2273-2277 | 35.4 | 266 |
| 113 | Structural and Na-ion conduction characteristics of Na3PSxSe4−x. *Journal of Materials Chemistry A*, **2016**, 4, 9044-9053 | 13 | 60 |
| 112 | A bio-facilitated synthetic route for nano-structured complex electrode materials. *Green Chemistry*, **2016**, 18, 2619-2624 | 10 | 13 |
| 111 | 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 |
| 110 | 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 |
| 109 | First-principles evaluation of multi-valent cation insertion into orthorhombic V2O5. *Chemical Communications*, **2015**, 51, 13619-22 | 5.8 | 120 |
| 108 | First-Principles Studies on Cation Dopants and Electrolyte\|Cathode Interphases for Lithium Garnets. *Chemistry of Materials*, **2015**, 27, 4040-4047 | 9.6 | 190 |
| 107 | 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 |
| 106 | The Intercalation Phase Diagram of Mg in V2O5 from First-Principles. *Chemistry of Materials*, **2015**, 27, 3733-3742 | 9.6 | 100 |
| 105 | Kinetics of Nanoparticle Interactions in Battery Electrodes. *Journal of the Electrochemical Society*, **2015**, 162, A965-A973 | 3.9 | 23 |
| 104 | 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 |
| 103 | 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 |
| 102 | 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 |
| 101 | Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. *Chemistry of Materials*, **2015**, 27, 6016-6021 | 9.6 | 351 |
| 100 | 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 |
| 99 | Design principles for solid-state lithium superionic conductors. *Nature Materials*, **2015**, 14, 1026-31 | 27 | 817 |

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| 98 | A new class of high capacity cation-disordered oxides for rechargeable lithium batteries: LiNiTiMo oxides. *Energy and Environmental Science*, **2015**, 8, 3255-3265 | 35.4 | 169 |
| 97 | Li-ion conductivity in Li9S3N. *Journal of Materials Chemistry A*, **2015**, 3, 20338-20344 | 13 | 22 |
| 96 | 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 |
| 95 | 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 |
| 94 | 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 |
| 93 | NaTiO2: a layered anode material for sodium-ion batteries. *Energy and Environmental Science*, **2015**, 8, 195-202 | 35.4 | 220 |
| 92 | Vacancy Ordering in O3-Type Layered Metal Oxide Sodium-Ion Battery Cathodes. *Physical Review Applied*, **2015**, 4, | 4.3 | 64 |
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