

# Shyue Ping Ong

## List of Publications by Year in descending order

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Version: 2024-02-01

149  
papers

29,953  
citations

9264

74  
h-index

9589

142  
g-index

158  
all docs

158  
docs citations

158  
times ranked

23464  
citing authors

#	ARTICLE	IF	CITATIONS
1	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. <i>APL Materials</i> , 2013, 1, .	5.1	6,913
2	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. <i>Computational Materials Science</i> , 2013, 68, 314-319.	3.0	2,392
3	Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials. <i>Energy and Environmental Science</i> , 2011, 4, 3680.	30.8	1,236
4	Design principles for solid-state lithium superionic conductors. <i>Nature Materials</i> , 2015, 14, 1026-1031.	27.5	1,079
5	Formation enthalpies by mixing GGA and GGA $+$ calculations. <i>Physical Review B</i> , 2011, 84, .	3.2	853
6	A high-throughput infrastructure for density functional theory calculations. <i>Computational Materials Science</i> , 2011, 50, 2295-2310.	3.0	787
7	$\text{Li}^{10}\text{Fe}^{2}\text{P}^{12}\text{O}_{20}$ Phase Diagram from First Principles Calculations. <i>Chemistry of Materials</i> , 2008, 20, 1798-1807.	6.7	621
8	First Principles Study of the $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ Lithium Super Ionic Conductor Material. <i>Chemistry of Materials</i> , 2012, 24, 15-17.	6.7	600
9	Surface energies of elemental crystals. <i>Scientific Data</i> , 2016, 3, 160080.	5.3	583
10	The thermodynamic scale of inorganic crystalline metastability. <i>Science Advances</i> , 2016, 2, e1600225.	10.3	565
11	Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals. <i>Chemistry of Materials</i> , 2019, 31, 3564-3572.	6.7	561
12	Phase stability, electrochemical stability and ionic conductivity of the $\text{Li}_{10}\text{M}^2\text{X}_{12}$ (M = Ge, Si, Sn, Al or P, and X = O, S or Se) family of superionic conductors. <i>Energy and Environmental Science</i> , 2013, 6, 148-156.	30.8	545
13	Performance and Cost Assessment of Machine Learning Interatomic Potentials. <i>Journal of Physical Chemistry A</i> , 2020, 124, 731-745.	2.5	428
14	Accuracy of density functional theory in predicting formation energies of ternary oxides from binary oxides and its implication on phase stability. <i>Physical Review B</i> , 2012, 85, .	3.2	380
15	FireWorks: a dynamic workflow system designed for high-throughput applications. <i>Concurrency Computation Practice and Experience</i> , 2015, 27, 5037-5059.	2.2	373
16	Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput <i>ab Initio</i> Calculations. <i>Chemistry of Materials</i> , 2011, 23, 3495-3508.	6.7	363
17	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. <i>Chemistry of Materials</i> , 2011, 23, 2979-2986.	6.7	337
18	A disordered rock salt anode for fast-charging lithium-ion batteries. <i>Nature</i> , 2020, 585, 63-67.	27.8	326

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19	The Materials Application Programming Interface (API): A simple, flexible and efficient API for materials data based on REpresentational State Transfer (REST) principles. Computational Materials Science, 2015, 97, 209-215.	3.0	322
20	A Critical Review of Machine Learning of Energy Materials. Advanced Energy Materials, 2020, 10, 1903242.	19.5	319
21	Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds. Physical Review B, 2010, 82, .	3.2	298
22	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
23	Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations. Journal of the Electrochemical Society, 2016, 163, A67-A74.	2.9	265
24	Design and synthesis of the superionic conductor Na <sub>10</sub> SnP <sub>2</sub> S <sub>12</sub> . Nature Communications, 2016, 7, 11009.	12.8	246
25	Direct visualization of the Jahn-Teller effect coupled to Na ordering in Na <sub>5/8</sub> MnO <sub>2</sub> . Nature Materials, 2014, 13, 586-592.	27.5	237
26	Thermal stabilities of delithiated olivine MPO <sub>4</sub> (M=Fe, Mn) cathodes investigated using first principles calculations. Electrochemistry Communications, 2010, 12, 427-430.	4.7	224
27	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
28	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	8.7	207
29	Room-Temperature All-solid-state Rechargeable Sodium-ion Batteries with a Cl-doped Na <sub>3</sub> PS <sub>4</sub> Superionic Conductor. Scientific Reports, 2016, 6, 33733.	3.3	205
30	Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations. Journal of Materials Chemistry, 2011, 21, 17147.	6.7	204
31	Role of Na <sup>+</sup> Interstitials and Dopants in Enhancing the Na <sup>+</sup> Conductivity of the Cubic Na <sub>3</sub> PS <sub>4</sub> Superionic Conductor. Chemistry of Materials, 2015, 27, 8318-8325.	6.7	202
32	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	5.3	201
33	First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery. Physical Review B, 2011, 84, .	3.2	191
34	Data-Driven First-Principles Methods for the Study and Design of Alkali Superionic Conductors. Chemistry of Materials, 2017, 29, 281-288.	6.7	190
35	Effect of Rb and Ta Doping on the Ionic Conductivity and Stability of the Garnet Li <sub>7+2x</sub> (La <sub>3-x</sub> Rb <sub>x</sub> )(Zr <sub>2</sub> Ta <sub>x</sub> ) <sub>2</sub> Superionic Conductor: A First Principles Investigation. Chemistry of Materials, 2013, 25, 3048-3055.	6.7	185
36	New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships. Journal of Materials Research, 2016, 31, 977-994.	2.6	180

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37	A Facile Mechanism for Recharging $\text{Li}_2\text{O}_2$ in $\text{Li}_2\text{O}$ Batteries. Chemistry of Materials, 2013, 25, 3328-3336.	6.7	179
38	Deep neural networks for accurate predictions of crystal stability. Nature Communications, 2018, 9, 3800.	12.8	178
39	Insights into the Performance Limits of the $\text{Li}_7\text{P}_3\text{S}_{11}$ Superionic Conductor: A Combined First-Principles and Experimental Study. ACS Applied Materials & Interfaces, 2016, 8, 7843-7853.	8.0	169
40	Nanoscale Stabilization of Sodium Oxides: Implications for $\text{Na}_2\text{O}$ Batteries. Nano Letters, 2014, 14, 1016-1020.	9.1	162
41	Low hole polaron migration barrier in lithium peroxide. Physical Review B, 2012, 85, .	3.2	158
42	A comparison of destabilization mechanisms of the layered $\text{Na}_x\text{MO}_2$ and $\text{Li}_x\text{MO}_2$ compounds upon alkali de-intercalation. Physical Chemistry Chemical Physics, 2012, 14, 15571.	2.8	158
43	From the computer to the laboratory: materials discovery and design using first-principles calculations. Journal of Materials Science, 2012, 47, 7317-7340.	3.7	154
44	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
45	Probing Solid-Solid Interfacial Reactions in All-Solid-State Sodium-Ion Batteries with First-Principles Calculations. Chemistry of Materials, 2018, 30, 163-173.	6.7	150
46	Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations. Chemistry of Materials, 2014, 26, 5208-5214.	6.7	149
47	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. Chemical Reviews, 2020, 120, 6977-7019.	47.7	145
48	Recharging lithium battery research with first-principles methods. MRS Bulletin, 2011, 36, 185-191.	3.5	143
49	Atomistic simulations of dislocation mobility in refractory high-entropy alloys and the effect of chemical short-range order. Nature Communications, 2021, 12, 4873.	12.8	138
50	Rational Composition Optimization of the Lithium-Rich $\text{Li}_3\text{OCl}$ $\text{Br}$ Anti-Perovskite Superionic Conductors. Chemistry of Materials, 2015, 27, 3749-3755. <a href="#">on in olivine <math>\text{LiMnPO}_4</math></a>	6.7	130
51	$\text{LiFePO}_4$ and $\text{LiFePO}_4$	3.2	128
52	Divalent-doped $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ sodium superionic conductor: Improving the ionic conductivity via simultaneously optimizing the phase and chemistry of the primary and secondary phases. Journal of Power Sources, 2017, 347, 229-237.	7.8	122
53	Revealing Nanoscale Solid-Solid Interfacial Phenomena for Long-Life and High-Energy All-Solid-State Batteries. ACS Applied Materials & Interfaces, 2019, 11, 43138-43145.	8.0	122
54	Grain boundary properties of elemental metals. Acta Materialia, 2020, 186, 40-49.	7.9	115

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55	Complex strengthening mechanisms in the NbMoTaW multi-principal element alloy. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	111
56	A stable cathode-solid electrolyte composite for high-voltage, long-cycle-life solid-state sodium-ion batteries. <i>Nature Communications</i> , 2021, 12, 1256.	12.8	110
57	Ultrafast ion transport at a cathode-electrolyte interface and its strong dependence on salt solvation. <i>Nature Energy</i> , 2020, 5, 578-586.	39.5	104
58	Understanding the Electrochemical Mechanisms Induced by Gradient Mg <sup>2+</sup> Distribution of Na-Rich Na <sub>3</sub> V <sub>2</sub> Mg(PO <sub>4</sub> ) <sub>3</sub> /C <sup>6.7</sup> for Sodium Ion Batteries. <i>Chemistry of Materials</i> , 2018, 30, 2498-2505.	6.7	102
59	Mining Unexplored Chemistries for Phosphors for High-Color-Quality White-Light-Emitting Diodes. <i>Joule</i> , 2018, 2, 914-926.	24.0	97
60	Enabling Thin and Flexible Solid-State Composite Electrolytes by the Scalable Solution Process. <i>ACS Applied Energy Materials</i> , 2019, 2, 6542-6550.	5.1	96
61	High-throughput computational X-ray absorption spectroscopy. <i>Scientific Data</i> , 2018, 5, 180151.	5.3	94
62	Thermal Stability and Reactivity of Cathode Materials for Li-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 7013-7021.	8.0	93
63	Data-Driven Discovery of Full-Visible-Spectrum Phosphor. <i>Chemistry of Materials</i> , 2019, 31, 6286-6294.	6.7	92
64	Engineering of K <sub>3</sub> YSi <sub>2</sub> O <sub>7</sub> To Tune Photoluminescence with Selected Activators and Site Occupancy. <i>Chemistry of Materials</i> , 2019, 31, 7770-7778.	6.7	89
65	New Insights into the Interphase between the Na Metal Anode and Sulfide Solid-State Electrolytes: A Joint Experimental and Computational Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 10076-10086.	8.0	86
66	Li <sub>3</sub> Y(PS <sub>4</sub> ) <sub>2</sub> and Li <sub>5</sub> PS <sub>4</sub> Cl <sub>2</sub> : New Lithium Superionic Conductors Predicted from Silver Thiophosphates using Efficiently Tiered Ab Initio Molecular Dynamics Simulations. <i>Chemistry of Materials</i> , 2017, 29, 2474-2484.	6.7	85
67	Learning properties of ordered and disordered materials from multi-fidelity data. <i>Nature Computational Science</i> , 2021, 1, 46-53.	8.0	85
68	Understanding the Electrochemical Properties of Naphthalene Diimide: Implication for Stable and High-Rate Lithium-Ion Battery Electrodes. <i>Chemistry of Materials</i> , 2018, 30, 3508-3517.	6.7	84
69	Anisotropic work function of elemental crystals. <i>Surface Science</i> , 2019, 687, 48-55.	1.9	84
70	Direct Observation of Halide Migration and its Effect on the Photoluminescence of Methylammonium Lead Bromide Perovskite Single Crystals. <i>Advanced Materials</i> , 2017, 29, 1703451.	21.0	83
71	Vacancy Ordering in $O_{3}$ -Type Layered Metal Oxide Sodium-Ion Battery Cathodes. <i>Physical Review Applied</i> , 2015, 4, .	3.8	82
72	Automated generation and ensemble-learned matching of X-ray absorption spectra. <i>Npj Computational Materials</i> , 2018, 4, .	8.7	82

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73	Accurate force field for molybdenum by machine learning large materials data. Physical Review Materials, 2017, 1, .	2.4	82
74	Electronic Structure Descriptor for the Discovery of Narrow-Band Red-Emitting Phosphors. Chemistry of Materials, 2016, 28, 4024-4031.	6.7	78
75	Tunable Lithium-Ion Transport in Mixed-Halide Argyrodites $\text{Li}_6\text{PS}_5\text{ClBr}_x$ : An Unusual Compositional Space. Chemistry of Materials, 2021, 33, 1435-1443.	6.7	78
76	A long-lasting dual-function electrolyte additive for stable lithium metal batteries. Nano Energy, 2020, 75, 104889.	16.0	77
77	Computational studies of solid-state alkali conduction in rechargeable alkali-ion batteries. NPG Asia Materials, 2016, 8, e254-e254.	7.9	73
78	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. Chemistry of Materials, 2013, 25, 2064-2074.	6.7	72
79	Accelerating materials science with high-throughput computations and machine learning. Computational Materials Science, 2019, 161, 143-150.	3.0	71
80	An electrostatic spectral neighbor analysis potential for lithium nitride. Npj Computational Materials, 2019, 5, .	8.7	69
81	Electrochemically induced amorphous-to-rock-salt phase transformation in niobium oxide electrode for Li-ion batteries. Nature Materials, 2022, 21, 795-803.	27.5	69
82	Water Contributes to Higher Energy Density and Cycling Stability of Prussian Blue Analogue Cathodes for Aqueous Sodium-Ion Batteries. Chemistry of Materials, 2019, 31, 5933-5942.	6.7	66
83	Quantum-accurate spectral neighbor analysis potential models for Ni-Mo binary alloys and fcc metals. Physical Review B, 2018, 98, .	3.2	65
84	Investigation of the Effect of Functional Group Substitutions on the Gas-Phase Electron Affinities and Ionization Energies of Room-Temperature Ionic Liquids Ions using Density Functional Theory. Electrochimica Acta, 2010, 55, 3804-3811.	5.2	64
85	Thermodynamics, Kinetics and Structural Evolution of $\mu\text{-LiVOPO}_4$ over Multiple Lithium Intercalation. Chemistry of Materials, 2016, 28, 1794-1805.	6.7	64
86	Predicting Thermal Quenching in Inorganic Phosphors. Chemistry of Materials, 2020, 32, 6256-6265.	6.7	64
87	Computational study of metallic dopant segregation and embrittlement at molybdenum grain boundaries. Acta Materialia, 2016, 117, 91-99.	7.9	63
88	Large scale computational screening and experimental discovery of novel materials for high temperature $\text{CO}_2$ capture. Energy and Environmental Science, 2016, 9, 1346-1360.	30.8	61
89	First-principles study of iron oxyfluorides and lithiation of FeOF. Physical Review B, 2013, 87, .	3.2	52
90	Studies of Functional Defects for Fast $\text{Na}^+$ Conduction in $\text{Na}_3\text{YPS}_4\text{Cl}_x$ with a Combined Experimental and Computational Approach. Advanced Functional Materials, 2019, 29, 1807951.	14.9	51

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91	A framework for quantifying uncertainty in DFT energy corrections. <i>Scientific Reports</i> , 2021, 11, 15496.	3.3	51
92	Elucidating Structure-Composition-Property Relationships of the $\hat{\Gamma}^2$ -SiAlON:Eu <sup>2+</sup> Phosphor. <i>Chemistry of Materials</i> , 2016, 28, 8622-8630.	6.7	50
93	KVOPO <sub>4</sub> : A New High Capacity Multielectron Na-ion Battery Cathode. <i>Advanced Energy Materials</i> , 2018, 8, 1800221.	19.5	50
94	Predictive modeling and design rules for solid electrolytes. <i>MRS Bulletin</i> , 2018, 43, 746-751.	3.5	47
95	Comparison of the polymorphs of VOPO <sub>4</sub> as multi-electron cathodes for rechargeable alkali-ion batteries. <i>Journal of Materials Chemistry A</i> , 2017, 5, 17421-17431.	10.3	46
96	Random Forest Models for Accurate Identification of Coordination Environments from X-Ray Absorption Near-Edge Structure. <i>Patterns</i> , 2020, 1, 100013.	5.9	46
97	Elucidating the Limit of Li Insertion into the Spinel Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> . , 2019, 1, 96-102.		45
98	Relating voltage and thermal safety in Li-ion battery cathodes: a high-throughput computational study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5942-5953.	2.8	44
99	Accelerating materials discovery with Bayesian optimization and graph deep learning. <i>Materials Today</i> , 2021, 51, 126-135.	14.2	44
100	Experimental and Computational Evaluation of a Sodium-Rich Anti-Perovskite for Solid State Electrolytes. <i>Journal of the Electrochemical Society</i> , 2016, 163, A2165-A2171.	2.9	43
101	First-Order Interfacial Transformations with a Critical Point: Breaking the Symmetry at a Symmetric Tilt Grain Boundary. <i>Physical Review Letters</i> , 2018, 120, 085702.	7.8	43
102	Bridging the gap between simulated and experimental ionic conductivities in lithium superionic conductors. <i>Materials Today Physics</i> , 2021, 21, 100463.	6.0	43
103	Molybdenum Substituted Vanadyl Phosphate $\hat{\Gamma}^2$ -VOPO <sub>4</sub> with Enhanced Two-Electron Transfer Reversibility and Kinetics for Lithium-Ion Batteries. <i>Chemistry of Materials</i> , 2016, 28, 3159-3170.	6.7	42
104	Cation-Size Mismatch as a Design Principle for Enhancing the Efficiency of Garnet Phosphors. <i>Chemistry of Materials</i> , 2020, 32, 3097-3108.	6.7	40
105	Interfacial Effects in $\hat{\Gamma}^2$ -Li <sub>x</sub> VOPO <sub>4</sub> and Evolution of the Electronic Structure. <i>Chemistry of Materials</i> , 2015, 27, 8211-8219.	6.7	37
106	Genetic algorithm-guided deep learning of grain boundary diagrams: Addressing the challenge of five degrees of freedom. <i>Materials Today</i> , 2020, 38, 49-57.	14.2	36
107	Effects of Transition-Metal Mixing on Na Ordering and Kinetics in Layered $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline">P\langle \text{mml:mi} \rangle 2 \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:math} \rangle$ Oxides. <i>Physical Review Applied</i> , 2017, 7, .	3.8	34
108	Efficient near-infrared phosphors discovered by parametrizing the Eu(II) 5d-to-4f energy gap. <i>Matter</i> , 2022, 5, 1924-1936.	10.0	31

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109	AtomSets as a hierarchical transfer learning framework for small and large materials datasets. Npj Computational Materials, 2021, 7, .	8.7	29
110	Design Principles for Aqueous Na-Ion Battery Cathodes. Chemistry of Materials, 2020, 32, 6875-6885.	6.7	28
111	Color tunable single-phase $\text{Eu}^{2+}$ and $\text{Ce}^{3+}$ co-activated $\text{Sr}_2\text{LiAlO}_4$ phosphors. Journal of Materials Chemistry C, 2019, 7, 7734-7744.	5.5	26
112	Vanadyl Phosphates $\text{AVOPO}_4$ (A = Li, Na, K) as Multielectron Cathodes for Alkali-Ion Batteries. Advanced Energy Materials, 2020, 10, 2002638.	19.5	26
113	First-principles insights on the magnetism of cubic $\text{SrTi}_{1-x}\text{Co}_x\text{O}_3$ . Applied Physics Letters, 2012, 100, 252904.	3.3	25
114	An integrated first principles and experimental investigation of the relationship between structural rigidity and quantum efficiency in phosphors for solid state lighting. Journal of Luminescence, 2016, 179, 297-305.	3.1	24
115	Multiprincipal Component $\text{P}_2\text{-Na}_{0.6}(\text{Ti}_{0.2}\text{Mn}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Ru}_{0.2})\text{O}_{12}$ as a High-Rate Cathode for Sodium-Ion Batteries. JACS, 2021, 1, 98-107.	2.2	22
116	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
117	Uniform second Li ion intercalation in solid state $\mu\text{-LiVOPO}_4$ . Applied Physics Letters, 2016, 109, .	3.3	20
118	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
119	Rational synthesis and electrochemical performance of $\text{LiVOPO}_4$ polymorphs. Journal of Materials Chemistry A, 2019, 7, 8423-8432.	10.3	20
120	Aqueous Stability of Alkali Superionic Conductors from First-Principles Calculations. Frontiers in Energy Research, 2016, 4, .	2.3	19
121	Role of Zr in strengthening $\text{MoSi}_2$ from density functional theory calculations. Acta Materialia, 2018, 145, 470-476.	7.9	17
122	Magnetism and Faraday Rotation in Oxygen-Deficient Polycrystalline and Single-Crystal Iron-Substituted Strontium Titanate. Physical Review Applied, 2017, 7, .	3.8	16
123	The Promise and Challenges of Quantum Computing for Energy Storage. Joule, 2018, 2, 810-813.	24.0	16
124	Correlated Octahedral Rotation and Organic Cation Reorientation Assist Halide Ion Migration in Lead Halide Perovskites. Chemistry of Materials, 2021, 33, 4672-4678.	6.7	16
125	Chlorine-Doped Perovskite Oxide: A Platinum-Free Cathode for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 35641-35652.	8.0	15
126	Inherent stochasticity during insulator-metal transition in $\text{VO}_2$ . Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	15



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127	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
128	$\text{La}^{1-x}\text{SiO}_2^{x-y}\text{N}_z$ ( $x = \text{Ca/Sr/Ba}$ ): Elucidating and Tuning the Structure and $\text{Eu}^{2+}$ Local Environments to Develop Full-Visible Spectrum Phosphors. Chemistry of Materials, 2022, 34, 4039-4049.	6.7	14
129	Design Principles for Cation-Mixed Sodium Solid Electrolytes. Advanced Energy Materials, 2021, 11, 2003196.	19.5	13
130	A Universal Machine Learning Model for Elemental Grain Boundary Energies. Scripta Materialia, 2022, 218, 114803.	5.2	12
131	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
132	Jahn-Teller distortion-driven robust blue-light-emitting perovskite nanoplatelets. Applied Materials Today, 2020, 20, 100668.	4.3	11
133	Structural Changes in a High-Energy Density $\text{VO}_2$ Cathode upon Heating and Li Cycling. ACS Applied Energy Materials, 2018, 1, 4514-4521.	5.1	10
134	Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project. , 2012, , .		8
135	Ab Initio Molecular Dynamics Studies of Fast Ion Conductors. , 2018, , 147-168.		8
136	Emergence of near-boundary segregation zones in face-centered cubic multiprincipal element alloys. Physical Review Materials, 2021, 5, .	2.4	7
137	Local environment rigidity and the evolution of optical properties in the green-emitting phosphor $\text{Ba}^{1-x}\text{Sr}^x\text{ScO}_2\text{F:Eu}^{2+}$ . Journal of Materials Chemistry C, 2022, 10, 2955-2964.	5.5	7
138	Morphology Control of Tantalum Carbide Nanoparticles through Dopant Additions. Journal of Physical Chemistry C, 2021, 125, 10665-10675.	3.1	6
139	Proton distribution visualization in perovskite nickelate devices utilizing nanofocused x rays. Physical Review Materials, 2021, 5, .	2.4	6
140	Role of Critical Oxygen Concentration in the $\text{Li}_3\text{PS}_4$ - $\text{O}_x$ Solid Electrolyte. ACS Applied Energy Materials, 2022, 5, 35-41.	5.1	6
141	Metal-insulator transition in $\text{V}_2\text{O}_3$ with intrinsic defects. Physical Review B, 2021, 103, .	3.2	5
142	Predicting the volumes of crystals. Computational Materials Science, 2018, 146, 184-192.	3.0	4
143	Creation of an XAS and EELS Spectroscopy Resource within the Materials Project using FEFF9. Microscopy and Microanalysis, 2017, 23, 208-209.	0.4	3
144	Correction to Insights into the Performance Limits of the $\text{Li}_7\text{P}_3\text{S}_{11}$ Superionic Conductor: A Combined First-Principles and Experimental Study. ACS Applied Materials & Interfaces, 2018, 10, 10598-10598.	8.0	3

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145	Exploring Frontiers in Research and Teaching: NanoEngineering and Chemical Engineering at UC San Diego. ACS Nano, 2020, 14, 9203-9216.	14.6	2
146	Battery Electrodes, Electrolytes, and Their Interfaces. , 2018, , 1-24.		1
147	Battery Electrodes, Electrolytes, and Their Interfaces. , 2019, , 1-24.		1
148	Publisher's Note: Accurate force field for molybdenum by machine learning large materials data [Phys. Rev. Materials <b>1</b> (2017)]. Physical Review Materials, 2018, 2, .	2.4	0
149	Battery Electrodes, Electrolytes, and Their Interfaces. , 2020, , 1231-1254.		0