Shyue Ping Ong

List of Publications by Citations

141 papers	19,560 citations	60 h-index	139 g-index
158 ext. papers	24,397 ext. citations	10.6 avg, IF	7.04 L-index

#	Paper	IF	Citations
141	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. *APL Materials*, **2013**, 1, 011002	5.7	4073
140	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. *Computational Materials Science*, **2013**, 68, 314-319	3.2	1435
139	Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials. *Energy and Environmental Science*, **2011**, 4, 3680	35.4	1078
138	Design principles for solid-state lithium superionic conductors. *Nature Materials*, **2015**, 14, 1026-31	27	817
137	A high-throughput infrastructure for density functional theory calculations. *Computational Materials Science*, **2011**, 50, 2295-2310	3.2	609
136	Formation enthalpies by mixing GGA and GGA + U calculations. *Physical Review B*, **2011**, 84,	3.3	607
135	Li–Be–P–O2 Phase Diagram from First Principles Calculations. *Chemistry of Materials*, **2008**, 20, 1798-1807	9.6	484
134	First Principles Study of the Li10GeP2S12 Lithium Super Ionic Conductor Material. *Chemistry of Materials*, **2012**, 24, 15-17	9.6	459
133	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
132	Surface energies of elemental crystals. *Scientific Data*, **2016**, 3, 160080	8.2	371
131	The thermodynamic scale of inorganic crystalline metastability. *Science Advances*, **2016**, 2, e1600225	14.3	352
130	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
129	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
128	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
127	Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds. *Physical Review B*, **2010**, 82,	3.3	251
126	FireWorks: a dynamic workflow system designed for high-throughput applications. *Concurrency Computation Practice and Experience*, **2015**, 27, 5037-5059	1.4	242
125	Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals. *Chemistry of Materials*, **2019**, 31, 3564-3572	9.6	219

124	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
123	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. *Journal of Physical Chemistry Letters*, **2015**, 6, 283-91	6.4	202
122	Design and synthesis of the superionic conductor Na10SnP2S12. *Nature Communications*, **2016**, 7, 11009	17.4	193
121	Direct visualization of the Jahn-Teller effect coupled to Na ordering in Na5/8MnO2. *Nature Materials*, **2014**, 13, 586-92	27	191
120	Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations. *Journal of the Electrochemical Society*, **2016**, 163, A67-A74	3.9	188
119	Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations. *Electrochemistry Communications*, **2010**, 12, 427-430	5.1	187
118	Performance and Cost Assessment of Machine Learning Interatomic Potentials. *Journal of Physical Chemistry A*, **2020**, 124, 731-745	2.8	185
117	First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery. *Physical Review B*, **2011**, 84,	3.3	174
116	Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations. *Journal of Materials Chemistry*, **2011**, 21, 17147		173
115	A Critical Review of Machine Learning of Energy Materials. *Advanced Energy Materials*, **2020**, 10, 1903242	21.8	155
114	A Facile Mechanism for Recharging Li2O2 in Li□O2 Batteries. *Chemistry of Materials*, **2013**, 25, 3328-3336	9.6	153
113	Room-Temperature All-solid-state Rechargeable Sodium-ion Batteries with a Cl-doped Na3PS4 Superionic Conductor. *Scientific Reports*, **2016**, 6, 33733	4.9	147
112	Low hole polaron migration barrier in lithium peroxide. *Physical Review B*, **2012**, 85,	3.3	145
111	Nanoscale stabilization of sodium oxides: implications for Na-O2 batteries. *Nano Letters*, **2014**, 14, 1016-20	11.5	144
110	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. *Computational Materials Science*, **2017**, 139, 140-152	3.2	142
109	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
108	Role of Na+ Interstitials and Dopants in Enhancing the Na+ Conductivity of the Cubic Na3PS4 Superionic Conductor. *Chemistry of Materials*, **2015**, 27, 8318-8325	9.6	137
107	A disordered rock salt anode for fast-charging lithium-ion batteries. *Nature*, **2020**, 585, 63-67	50.4	137

106	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
105	New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships. *Journal of Materials Research*, **2016**, 31, 977-994	2.5	133
104	Insights into the Performance Limits of the Li7P3S11 Superionic Conductor: A Combined First-Principles and Experimental Study. *ACS Applied Materials & Interfaces*, **2016**, 8, 7843-53	9.5	130
103	Recharging lithium battery research with first-principles methods. *MRS Bulletin*, **2011**, 36, 185-191	3.2	130
102	From the computer to the laboratory: materials discovery and design using first-principles calculations. *Journal of Materials Science*, **2012**, 47, 7317-7340	4.3	129
101	The Electrolyte Genome project: A big data approach in battery materials discovery. *Computational Materials Science*, **2015**, 103, 56-67	3.2	123
100	Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations. *Chemistry of Materials*, **2014**, 26, 5208-5214	9.6	121
99	Data-Driven First-Principles Methods for the Study and Design of Alkali Superionic Conductors. *Chemistry of Materials*, **2017**, 29, 281-288	9.6	120
98	Deep neural networks for accurate predictions of crystal stability. *Nature Communications*, **2018**, 9, 3800	17.4	119
97	Comparison of small polaron migration and phase separation in olivine LiMnPO4 and LiFePO4 using hybrid density functional theory. *Physical Review B*, **2011**, 83,	3.3	117
96	Probing Solid□Solid Interfacial Reactions in All-Solid-State Sodium-Ion Batteries with First-Principles Calculations. *Chemistry of Materials*, **2018**, 30, 163-173	9.6	104
95	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. *Scientific Data*, **2019**, 6, 86	8.2	92
94	Rational Composition Optimization of the Lithium-Rich Li3OCl1□Brx Anti-Perovskite Superionic Conductors. *Chemistry of Materials*, **2015**, 27, 3749-3755	9.6	92
93	Divalent-doped Na3Zr2Si2PO12 natrium 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	8.9	77
92	Mining Unexplored Chemistries for Phosphors for High-Color-Quality White-Light-Emitting Diodes. *Joule*, **2018**, 2, 914-926	27.8	69
91	Li3Y(PS4)2 and Li5PS4Cl2: New Lithium Superionic Conductors Predicted from Silver Thiophosphates using Efficiently Tiered Ab Initio Molecular Dynamics Simulations. *Chemistry of Materials*, **2017**, 29, 2474-2484	9.6	68
90	Direct Observation of Halide Migration and its Effect on the Photoluminescence of Methylammonium Lead Bromide Perovskite Single Crystals. *Advanced Materials*, **2017**, 29, 1703451	24	68
89	Understanding the Electrochemical Mechanisms Induced by Gradient Mg2+ Distribution of Na-Rich Na3+xV2□Mgx(PO4)3/C for Sodium Ion Batteries. *Chemistry of Materials*, **2018**, 30, 2498-2505	9.6	68

88	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. *Chemical Reviews*, **2020**, 120, 6977-7019	68.1	68
87	Thermal Stability and Reactivity of Cathode Materials for Li-Ion Batteries. *ACS Applied Materials & Interfaces*, **2016**, 8, 7013-21	9.5	66
86	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. *Chemistry of Materials*, **2013**, 25, 2064-2074	9.6	65
85	Vacancy Ordering in O3-Type Layered Metal Oxide Sodium-Ion Battery Cathodes. *Physical Review Applied*, **2015**, 4,	4.3	64
84	Electronic Structure Descriptor for the Discovery of Narrow-Band Red-Emitting Phosphors. *Chemistry of Materials*, **2016**, 28, 4024-4031	9.6	64
83	High-throughput computational X-ray absorption spectroscopy. *Scientific Data*, **2018**, 5, 180151	8.2	63
82	New Insights into the Interphase between the Na Metal Anode and Sulfide Solid-State Electrolytes: A Joint Experimental and Computational Study. *ACS Applied Materials & Interfaces*, **2018**, 10, 10076-10086	9.5	62
81	Understanding the Electrochemical Properties of Naphthalene Diimide: Implication for Stable and High-Rate Lithium-Ion Battery Electrodes. *Chemistry of Materials*, **2018**, 30, 3508-3517	9.6	60
80	Computational studies of solid-state alkali conduction in rechargeable alkali-ion batteries. *NPG Asia Materials*, **2016**, 8, e254-e254	10.3	57
79	Revealing Nanoscale Solid-Solid Interfacial Phenomena for Long-Life and High-Energy All-Solid-State Batteries. *ACS Applied Materials & Interfaces*, **2019**, 11, 43138-43145	9.5	57
78	Thermodynamics, Kinetics and Structural Evolution of □LiVOPO4 over Multiple Lithium Intercalation. *Chemistry of Materials*, **2016**, 28, 1794-1805	9.6	56
77	Accurate force field for molybdenum by machine learning large materials data. *Physical Review Materials*, **2017**, 1,	3.2	55
76	Automated generation and ensemble-learned matching of X-ray absorption spectra. *Npj Computational Materials*, **2018**, 4,	10.9	54
75	Data-Driven Discovery of Full-Visible-Spectrum Phosphor. *Chemistry of Materials*, **2019**, 31, 6286-6294	9.6	54
74	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	6.7	53
73	Engineering of K3YSi2O7 To Tune Photoluminescence with Selected Activators and Site Occupancy. *Chemistry of Materials*, **2019**, 31, 7770-7778	9.6	50
72	An electrostatic spectral neighbor analysis potential for lithium nitride. *Npj Computational Materials* , **2019**, 5,	10.9	44
71	Large scale computational screening and experimental discovery of novel materials for high temperature CO2 capture. *Energy and Environmental Science*, **2016**, 9, 1346-1360	35.4	43

70	First-principles study of iron oxyfluorides and lithiation of FeOF. *Physical Review B*, **2013**, 87,	3.3	43
69	Computational study of metallic dopant segregation and embrittlement at molybdenum grain boundaries. *Acta Materialia*, **2016**, 117, 91-99	8.4	43
68	Enabling Thin and Flexible Solid-State Composite Electrolytes by the Scalable Solution Process. *ACS Applied Energy Materials*, **2019**, 2, 6542-6550	6.1	42
67	Grain boundary properties of elemental metals. *Acta Materialia*, **2020**, 186, 40-49	8.4	42
66	Anisotropic work function of elemental crystals. *Surface Science*, **2019**, 687, 48-55	1.8	41
65	A long-lasting dual-function electrolyte additive for stable lithium metal batteries. *Nano Energy*, **2020**, 75, 104889	17.1	38
64	Relating voltage and thermal safety in Li-ion battery cathodes: a high-throughput computational study. *Physical Chemistry Chemical Physics*, **2015**, 17, 5942-53	3.6	37
63	Elucidating Structure□Composition□Property Relationships of the □SiAlON:Eu2+ Phosphor. *Chemistry of Materials*, **2016**, 28, 8622-8630	9.6	36
62	Ultrafast ion transport at a cathode□electrolyte interface and its strong dependence on salt solvation. *Nature Energy*, **2020**, 5, 578-586	62.3	35
61	Complex strengthening mechanisms in the NbMoTaW multi-principal element alloy. *Npj Computational Materials*, **2020**, 6,	10.9	35
60	Comparison of the polymorphs of VOPO4 as multi-electron cathodes for rechargeable alkali-ion batteries. *Journal of Materials Chemistry A*, **2017**, 5, 17421-17431	13	35
59	Accelerating materials science with high-throughput computations and machine learning. *Computational Materials Science*, **2019**, 161, 143-150	3.2	35
58	Quantum-accurate spectral neighbor analysis potential models for Ni-Mo binary alloys and fcc metals. *Physical Review B*, **2018**, 98,	3.3	35
57	Interfacial Effects in □LixVOPO4 and Evolution of the Electronic Structure. *Chemistry of Materials*, **2015**, 27, 8211-8219	9.6	33
56	Learning properties of ordered and disordered materials from multi-fidelity data. *Nature Computational Science*, **2021**, 1, 46-53		32
55	First-Order Interfacial Transformations with a Critical Point: Breaking the Symmetry at a Symmetric Tilt Grain Boundary. *Physical Review Letters*, **2018**, 120, 085702	7.4	31
54	Molybdenum Substituted Vanadyl Phosphate □VOPO4 with Enhanced Two-Electron Transfer Reversibility and Kinetics for Lithium-Ion Batteries. *Chemistry of Materials*, **2016**, 28, 3159-3170	9.6	31
53	A stable cathode-solid electrolyte composite for high-voltage, long-cycle-life solid-state sodium-ion batteries. *Nature Communications*, **2021**, 12, 1256	17.4	31

52	Predictive modeling and design rules for solid electrolytes. *MRS Bulletin*, **2018**, 43, 746-751	3.2	31
51	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	9.6	30
50	Studies of Functional Defects for Fast Na-Ion Conduction in Na3□PS4□Clx with a Combined Experimental and Computational Approach. *Advanced Functional Materials*, **2019**, 29, 1807951	15.6	30
49	Experimental and Computational Evaluation of a Sodium-Rich Anti-Perovskite for Solid State Electrolytes. *Journal of the Electrochemical Society*, **2016**, 163, A2165-A2171	3.9	29
48	Elucidating the Limit of Li Insertion into the Spinel Li4Ti5O12 **2019**, 1, 96-102		28
47	KVOPO4: A New High Capacity Multielectron Na-Ion Battery Cathode. *Advanced Energy Materials*, **2018**, 8, 1800221	21.8	28
46	Effects of Transition-Metal Mixing on Na Ordering and Kinetics in Layered P2 Oxides. *Physical Review Applied*, **2017**, 7,	4.3	26
45	Random Forest Models for Accurate Identification of Coordination Environments from X-Ray Absorption Near-Edge Structure. *Patterns*, **2020**, 1, 100013	5.1	26
44	Tunable Lithium-Ion Transport in Mixed-Halide Argyrodites Li6□PS5□ClBrx: An Unusual Compositional Space. *Chemistry of Materials*, **2021**, 33, 1435-1443	9.6	26
43	Predicting Thermal Quenching in Inorganic Phosphors. *Chemistry of Materials*, **2020**, 32, 6256-6265	9.6	25
42	First-principles insights on the magnetism of cubic SrTi1□CoxO3□*Applied Physics Letters*, **2012**, 100, 252904	3.4	23
41	Genetic algorithm-guided deep learning of grain boundary diagrams: Addressing the challenge of five degrees of freedom. *Materials Today*, **2020**, 38, 49-57	21.8	21
40	Atomistic simulations of dislocation mobility in refractory high-entropy alloys and the effect of chemical short-range order. *Nature Communications*, **2021**, 12, 4873	17.4	21
39	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	3.8	19
38	Recent advances and applications of deep learning methods in materials science. *Npj Computational Materials*, **2022**, 8,	10.9	19
37	Color tunable single-phase Eu2+ and Ce3+ co-activated Sr2LiAlO4 phosphors. *Journal of Materials Chemistry C*, **2019**, 7, 7734-7744	7.1	17
36	Uniform second Li ion intercalation in solid state ?-LiVOPO4. *Applied Physics Letters*, **2016**, 109, 053904	3.4	17
35	Rational synthesis and electrochemical performance of LiVOPO4 polymorphs. *Journal of Materials Chemistry A*, **2019**, 7, 8423-8432	13	16

34	Harnessing the Materials Project for machine-learning and accelerated discovery. *MRS Bulletin*, **2018**, 43, 664-669	3.2	16
33	Aqueous Stability of Alkali Superionic Conductors from First-Principles Calculations. *Frontiers in Energy Research*, **2016**, 4,	3.8	15
32	Cation-Size Mismatch as a Design Principle for Enhancing the Efficiency of Garnet Phosphors. *Chemistry of Materials*, **2020**, 32, 3097-3108	9.6	13
31	Role of Zr in strengthening MoSi2 from density functional theory calculations. *Acta Materialia*, **2018** , 145, 470-476	8.4	13
30	Chlorine-Doped Perovskite Oxide: A Platinum-Free Cathode for Dye-Sensitized Solar Cells. *ACS Applied Materials & Interfaces*, **2019**, 11, 35641-35652	9.5	11
29	Vanadyl Phosphates AxVOPO4 (A = Li, Na, K) as Multielectron Cathodes for Alkali-Ion Batteries. *Advanced Energy Materials*, **2020**, 10, 2002638	21.8	11
28	Bridging the gap between simulated and experimental ionic conductivities in lithium superionic conductors. *Materials Today Physics*, **2021**, 21, 100463	8	11
27	Magnetism and Faraday Rotation in Oxygen-Deficient Polycrystalline and Single-Crystal Iron-Substituted Strontium Titanate. *Physical Review Applied*, **2017**, 7,	4.3	10
26	Design Principles for Aqueous Na-Ion Battery Cathodes. *Chemistry of Materials*, **2020**, 32, 6875-6885	9.6	10
25	A framework for quantifying uncertainty in DFT energy corrections. *Scientific Reports*, **2021**, 11, 15496	4.9	8
24	Electrochemically induced amorphous-to-rock-salt phase transformation in niobium oxide electrode for Li-ion batteries.. *Nature Materials*, **2022**,	27	8
23	Jahn□eller distortion-driven robust blue-light-emitting perovskite nanoplatelets. *Applied Materials Today*, **2020**, 20, 100668	6.6	7
22	Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project **2012**,		7
21	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools **2018**, 1-34		7
20	Structural Changes in a High-Energy Density VO2F Cathode upon Heating and Li Cycling. *ACS Applied Energy Materials*, **2018**, 1, 4514-4521	6.1	7
19	Design Principles for Cation-Mixed Sodium Solid Electrolytes. *Advanced Energy Materials*, **2021**, 11, 2003126	27.8	6
18	The Promise and Challenges of Quantum Computing for Energy Storage. *Joule*, **2018**, 2, 810-813	27.8	6
17	Multiprincipal Component P2-Na(TiMnCoNiRu)O as a High-Rate Cathode for Sodium-Ion Batteries. *Jacs Au*, **2021**, 1, 98-107		5

16	AtomSets as a hierarchical transfer learning framework for small and large materials datasets. *Npj Computational Materials*, **2021**, 7,	10.9	4
15	Database of ab initio L-edge X-ray absorption near edge structure. *Scientific Data*, **2021**, 8, 153	8.2	4
14	Ab Initio Molecular Dynamics Studies of Fast Ion Conductors **2018**, 147-168		4
13	Accelerating materials discovery with Bayesian optimization and graph deep learning. *Materials Today*, **2021**,	21.8	4
12	Creation of an XAS and EELS Spectroscopy Resource within the Materials Project using FEFF9. *Microscopy and Microanalysis*, **2017**, 23, 208-209	0.5	3
11	Correlated Octahedral Rotation and Organic Cation Reorientation Assist Halide Ion Migration in Lead Halide Perovskites. *Chemistry of Materials*, **2021**, 33, 4672-4678	9.6	3
10	Inherent stochasticity during insulator-metal transition in VO. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
9	Predicting the volumes of crystals. *Computational Materials Science*, **2018**, 146, 184-192	3.2	2
8	A Universal Machine Learning Model for Elemental Grain Boundary Energies. *Scripta Materialia*, **2022**, 218, 114803	5.6	2
7	Role of Critical Oxygen Concentration in the □Li3PS4□Ox Solid Electrolyte. *ACS Applied Energy Materials*, **2022**, 5, 35-41	6.1	1
6	Morphology Control of Tantalum Carbide Nanoparticles through Dopant Additions. *Journal of Physical Chemistry C*, **2021**, 125, 10665-10675	3.8	1
5	Battery Electrodes, Electrolytes, and Their Interfaces **2019**, 1-24		1
4	Battery Electrodes, Electrolytes, and Their Interfaces **2018**, 1-24		1
3	Proton distribution visualization in perovskite nickelate devices utilizing nanofocused x rays. *Physical Review Materials*, **2021**, 5,	3.2	1
2	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools **2020**, 1751-1784		0
1	Battery Electrodes, Electrolytes, and Their Interfaces **2020**, 1231-1254		