Shyue Ping Ong

List of Publications by Year
in descending order

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Version: 2024-02-01

		9264	9589
149	29,953	74	142
papers	citations	h-index	g-index

158	158	158	23464
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Role of Critical Oxygen Concentration in the Î²-Li₃PS_{4â€“x}O_x Solid Electrolyte. ACS Applied Energy Materials, 2022, 5, 35-41.	5.1	6
2	Local environment rigidity and the evolution of optical properties in the green-emitting phosphor Ba_{1â^’x}Sr_xScO₂F:Eu²⁺. Journal of Materials Chemistry C, 2022, 10, 2955-2964.	5.5	7
3	M_xLa_{1â€“x}SiO_{2â€“y}N_z (M = Ca/Sr/Ba): Elucidating and Tuning the Structure and Eu²⁺ Local Environments to Develop Full-Visible Spectrum Phosphors. Chemistry of Materials, 2022, 34, 4039-4049.	6.7	14
4	Recent advances and applications of deep learning methods in materials science. Npj Computational Materials, 2022, 8, .	8.7	207
5	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
6	Efficient near-infrared phosphors discovered by parametrizing the Eu(II) 5d-to-4f energy gap. Matter, 2022, 5, 1924-1936.	10.0	31
7	A Universal Machine Learning Model for Elemental Grain Boundary Energies. Scripta Materialia, 2022, 218, 114803.	5.2	12
8	Multiprincipal Component P2-Na_{0.6}(Ti_{0.2}Mn_{0.2}Co_{0.2}Ni_{0.2}Ru_{0.2})O₂ as a High-Rate Cathode for Sodium-Ion Batteries. Jacs Au, 2021, 1, 98-107.	10.9	22
9	Design Principles for Cationâ€Mixed Sodium Solid Electrolytes. Advanced Energy Materials, 2021, 11, 2003196.	19.5	13
10	A stable cathode-solid electrolyte composite for high-voltage, long-cycle-life solid-state sodium-ion batteries. Nature Communications, 2021, 12, 1256.	12.8	110
11	Metal-insulator transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> with intrinsic defects. Physical Review B, 2021, 103, .	3.2	5
12	Tunable Lithium-Ion Transport in Mixed-Halide Argyrodites Li_{6â€“x}PS_{5â€“x}ClBr_x: An Unusual Compositional Space. Chemistry of Materials, 2021, 33, 1435-1443.	6.7	78
13	Morphology Control of Tantalum Carbide Nanoparticles through Dopant Additions. Journal of Physical Chemistry C, 2021, 125, 10665-10675.	3.1	6
14	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
15	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
16	A framework for quantifying uncertainty in DFT energy corrections. Scientific Reports, 2021, 11, 15496.	3.3	51
17	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
18	Inherent stochasticity during insulatorâ€“metal transition in VO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	15

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19	Proton distribution visualization in perovskite nickelate devices utilizing nanofocused x rays. Physical Review Materials, 2021, 5, .	2.4	6
20	Accelerating materials discovery with Bayesian optimization and graph deep learning. Materials Today, 2021, 51, 126-135.	14.2	44
21	Bridging the gap between simulated and experimental ionic conductivities in lithium superionic conductors. Materials Today Physics, 2021, 21, 100463.	6.0	43
22	Learning properties of ordered and disordered materials from multi-fidelity data. Nature Computational Science, 2021, 1, 46-53.	8.0	85
23	AtomSets as a hierarchical transfer learning framework for small and large materials datasets. Npj Computational Materials, 2021, 7, .	8.7	29
24	Emergence of near-boundary segregation zones in face-centered cubic multiprincipal element alloys. Physical Review Materials, 2021, 5, .	2.4	7
25	Grain boundary properties of elemental metals. Acta Materialia, 2020, 186, 40-49.	7.9	115
26	Design Principles for Aqueous Na-Ion Battery Cathodes. Chemistry of Materials, 2020, 32, 6875-6885.	6.7	28
27	Exploring Frontiers in Research and Teaching: NanoEngineering and Chemical Engineering at UC San Diego. ACS Nano, 2020, 14, 9203-9216.	14.6	2
28	Vanadyl Phosphates A_xVOPO₄ (A = Li, Na, K) as Multielectron Cathodes for Alkaliâ€ion Batteries. Advanced Energy Materials, 2020, 10, 2002638.	19.5	26
29	A disordered rock salt anode for fast-charging lithium-ion batteries. Nature, 2020, 585, 63-67.	27.8	326
30	A long-lasting dual-function electrolyte additive for stable lithium metal batteries. Nano Energy, 2020, 75, 104889.	16.0	77
31	Jahnâ€“Teller distortion-driven robust blue-light-emitting perovskite nanoplatelets. Applied Materials Today, 2020, 20, 100668.	4.3	11
32	Cation-Size Mismatch as a Design Principle for Enhancing the Efficiency of Garnet Phosphors. Chemistry of Materials, 2020, 32, 3097-3108.	6.7	40
33	Ultrafast ion transport at a cathodeâ€“electrolyte interface and its strong dependence on salt solvation. Nature Energy, 2020, 5, 578-586.	39.5	104
34	Predicting Thermal Quenching in Inorganic Phosphors. Chemistry of Materials, 2020, 32, 6256-6265.	6.7	64
35	Complex strengthening mechanisms in the NbMoTaW multi-principal element alloy. Npj Computational Materials, 2020, 6, .	8.7	111
36	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	2.5	428

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37	A Critical Review of Machine Learning of Energy Materials. Advanced Energy Materials, 2020, 10, 1903242.	19.5	319
38	Genetic algorithm-guided deep learning of grain boundary diagrams: Addressing the challenge of five degrees of freedom. Materials Today, 2020, 38, 49-57.	14.2	36
39	Random Forest Models for Accurate Identification of Coordination Environments from X-Ray Absorption Near-Edge Structure. Patterns, 2020, 1, 100013.	5.9	46
40	Rechargeable Alkali-Ion Battery Materials: Theory and Computation. Chemical Reviews, 2020, 120, 6977-7019.	47.7	145
41	Battery Electrodes, Electrolytes, and Their Interfaces. , 2020, , 1231-1254.		0
42	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2020, , 1751-1784.		14
43	Engineering of K₃YSi₂O₇ To Tune Photoluminescence with Selected Activators and Site Occupancy. Chemistry of Materials, 2019, 31, 7770-7778.	6.7	89
44	Enabling Thin and Flexible Solid-State Composite Electrolytes by the Scalable Solution Process. ACS Applied Energy Materials, 2019, 2, 6542-6550.	5.1	96
45	Data-Driven Discovery of Full-Visible-Spectrum Phosphor. Chemistry of Materials, 2019, 31, 6286-6294.	6.7	92
46	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
47	An electrostatic spectral neighbor analysis potential for lithium nitride. Npj Computational Materials, 2019, 5, .	8.7	69
48	Revealing Nanoscale Solidâ€“Solid Interfacial Phenomena for Long-Life and High-Energy All-Solid-State Batteries. ACS Applied Materials & Interfaces, 2019, 11, 43138-43145.	8.0	122
49	Chlorine-Doped Perovskite Oxide: A Platinum-Free Cathode for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2019, 11, 35641-35652.	8.0	15
50	Elucidating the Limit of Li Insertion into the Spinel Li₄Ti₅O₁₂. , 2019, 1, 96-102.		45
51	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	5.3	201
52	Color tunable single-phase Eu²⁺and Ce³⁺co-activated Sr₂LiAlO₄phosphors. Journal of Materials Chemistry C, 2019, 7, 7734-7744.	5.5	26
53	Anisotropic work function of elemental crystals. Surface Science, 2019, 687, 48-55.	1.9	84
54	Rational synthesis and electrochemical performance of LiVOPO₄ polymorphs. Journal of Materials Chemistry A, 2019, 7, 8423-8432.	10.3	20

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55	Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals. Chemistry of Materials, 2019, 31, 3564-3572.	6.7	561
56	Studies of Functional Defects for Fast Naâ€Ion Conduction in Na_{3â^'}_yPS_{4â^'}_xCl_x with a Combined Experimental and Computational Approach. Advanced Functional Materials, 2019, 29, 1807951.	14.9	51
57	Battery Electrodes, Electrolytes, and Their Interfaces. , 2019, , 1-24.		1
58	Accelerating materials science with high-throughput computations and machine learning. Computational Materials Science, 2019, 161, 143-150.	3.0	71
59	First-Order Interfacial Transformations with a Critical Point: Breaking the Symmetry at a Symmetric Tilt Grain Boundary. Physical Review Letters, 2018, 120, 085702.	7.8	43
60	Understanding the Electrochemical Mechanisms Induced by Gradient Mg²⁺ Distribution of Na-Rich Na_{3+x}V_{2â€“x}Mg_x(PO₄)₃/C for Sodium Ion Batteries. Chemistry of Materials, 2018, 30, 2498-2505.	6.7	102
61	Predicting the volumes of crystals. Computational Materials Science, 2018, 146, 184-192.	3.0	4
62	Mining Unexplored Chemistries for Phosphors for High-Color-Quality White-Light-Emitting Diodes. Joule, 2018, 2, 914-926.	24.0	97
63	Role of Zr in strengthening MoSi2 from density functional theory calculations. Acta Materialia, 2018, 145, 470-476.	7.9	17
64	Understanding the Electrochemical Properties of Naphthalene Diimide: Implication for Stable and High-Rate Lithium-Ion Battery Electrodes. Chemistry of Materials, 2018, 30, 3508-3517.	6.7	84
65	Automated generation and ensemble-learned matching of X-ray absorption spectra. Npj Computational Materials, 2018, 4, .	8.7	82
66	Correction to Insights into the Performance Limits of the Li7P3S11 Superionic Conductor: A Combined First-Principles and Experimental Study. ACS Applied Materials & Interfaces, 2018, 10, 10598-10598.	8.0	3
67	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.	8.0	86
68	Probing Solidâ€“Solid Interfacial Reactions in All-Solid-State Sodium-Ion Batteries with First-Principles Calculations. Chemistry of Materials, 2018, 30, 163-173.	6.7	150
69	Ab Initio Molecular Dynamics Studies of Fast Ion Conductors. , 2018, , 147-168.		8
70	Battery Electrodes, Electrolytes, and Their Interfaces. , 2018, , 1-24.		1
71	The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools. , 2018, , 1-34.		11
72	Predictive modeling and design rules for solid electrolytes. MRS Bulletin, 2018, 43, 746-751.	3.5	47

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73	Deep neural networks for accurate predictions of crystal stability. Nature Communications, 2018, 9, 3800.	12.8	178
74	Quantum-accurate spectral neighbor analysis potential models for Ni-Mo binary alloys and fcc metals. Physical Review B, 2018, 98, .	3.2	65
75	Harnessing the Materials Project for machine-learning and accelerated discovery. MRS Bulletin, 2018, 43, 664-669.	3.5	20
76	Structural Changes in a High-Energy Density VO₂F Cathode upon Heating and Li Cycling. ACS Applied Energy Materials, 2018, 1, 4514-4521.	5.1	10
77	The Promise and Challenges of Quantum Computing for Energy Storage. Joule, 2018, 2, 810-813.	24.0	16
78	KVOPO₄: A New High Capacity Multielectron Naâ€ion Battery Cathode. Advanced Energy Materials, 2018, 8, 1800221.	19.5	50
79	High-throughput computational X-ray absorption spectroscopy. Scientific Data, 2018, 5, 180151.	5.3	94
80	Publisher's Note: Accurate force field for molybdenum by machine learning large materials data [Phys. Rev. Materials 1 , 043603 (2017)]. Physical Review Materials, 2018, 2, .	2.4	0
81	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.	7.8	122
82	Magnetism and Faraday Rotation in Oxygen-Deficient Polycrystalline and Single-Crystal Iron-Substituted Strontium Titanate. Physical Review Applied, 2017, 7, .	3.8	16
83	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.	6.7	85
84	Direct Observation of Halide Migration and its Effect on the Photoluminescence of Methylammonium Lead Bromide Perovskite Single Crystals. Advanced Materials, 2017, 29, 1703451.	21.0	83
85	Comparison of the polymorphs of VOPO₄ as multi-electron cathodes for rechargeable alkali-ion batteries. Journal of Materials Chemistry A, 2017, 5, 17421-17431.	10.3	46
86	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
87	Effects of Transition-Metal Mixing on Na Ordering and Kinetics in Layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>P</mml:mi><mml:mn>2</mml:mn></mml:math> Oxides. Physical Review Applied, 2017, 7, .	3.8	34
88	Data-Driven First-Principles Methods for the Study and Design of Alkali Superionic Conductors. Chemistry of Materials, 2017, 29, 281-288.	6.7	190
89	Creation of an XAS and EELS Spectroscopy Resource within the Materials Project using FEFF9. Microscopy and Microanalysis, 2017, 23, 208-209.	0.4	3
90	Accurate force field for molybdenum by machine learning large materials data. Physical Review Materials, 2017, 1, .	2.4	82

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91	Aqueous Stability of Alkali Superionic Conductors from First-Principles Calculations. Frontiers in Energy Research, 2016, 4, .	2.3	19
92	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
93	Uniform second Li ion intercalation in solid state Ïµ-LiVOPO4. Applied Physics Letters, 2016, 109, .	3.3	20
94	Molybdenum Substituted Vanadyl Phosphate Îµ-VOPO₄ with Enhanced Two-Electron Transfer Reversibility and Kinetics for Lithium-Ion Batteries. Chemistry of Materials, 2016, 28, 3159-3170.	6.7	42
95	Electronic Structure Descriptor for the Discovery of Narrow-Band Red-Emitting Phosphors. Chemistry of Materials, 2016, 28, 4024-4031.	6.7	78
96	Computational study of metallic dopant segregation and embrittlement at molybdenum grain boundaries. Acta Materialia, 2016, 117, 91-99.	7.9	63
97	Experimental and Computational Evaluation of a Sodium-Rich Anti-Perovskite for Solid State Electrolytes. Journal of the Electrochemical Society, 2016, 163, A2165-A2171.	2.9	43
98	The thermodynamic scale of inorganic crystalline metastability. Science Advances, 2016, 2, e1600225.	10.3	565
99	Elucidating Structureâ€“Compositionâ€“Property Relationships of the Î²-SiAlON:Eu²⁺ Phosphor. Chemistry of Materials, 2016, 28, 8622-8630.	6.7	50
100	Design and synthesis of the superionic conductor Na10SnP2S12. Nature Communications, 2016, 7, 11009.	12.8	246
101	Surface energies of elemental crystals. Scientific Data, 2016, 3, 160080.	5.3	583
102	Room-Temperature All-solid-state Rechargeable Sodium-ion Batteries with a Cl-doped Na3PS4 Superionic Conductor. Scientific Reports, 2016, 6, 33733.	3.3	205
103	Computational studies of solid-state alkali conduction in rechargeable alkali-ion batteries. NPG Asia Materials, 2016, 8, e254-e254.	7.9	73
104	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
105	Large scale computational screening and experimental discovery of novel materials for high temperature CO₂ capture. Energy and Environmental Science, 2016, 9, 1346-1360.	30.8	61
106	Thermal Stability and Reactivity of Cathode Materials for Li-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 7013-7021.	8.0	93
107	Thermodynamics, Kinetics and Structural Evolution of Îµ-LiVOPO4 over Multiple Lithium Intercalation. Chemistry of Materials, 2016, 28, 1794-1805.	6.7	64
108	Insights into the Performance Limits of the Li₇P₃S₁₁ Superionic Conductor: A Combined First-Principles and Experimental Study. ACS Applied Materials & Interfaces, 2016, 8, 7843-7853.	8.0	169

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109	Elastic Properties of Alkali Superionic Conductor Electrolytes from First Principles Calculations. Journal of the Electrochemical Society, 2016, 163, A67-A74.	2.9	265
110	Vacancy Ordering in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>O</mml:mi><mml:mn>3</mml:mn></mml:math> -Type Layered Metal Oxide Sodium-Ion Battery Cathodes. Physical Review Applied, 2015, 4, .	3.8	82
111	FireWorks: a dynamic workflow system designed for highâ€throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
112	Interfacial Effects in Îµ-Li_xVOPO₄ and Evolution of the Electronic Structure. Chemistry of Materials, 2015, 27, 8211-8219.	6.7	37
113	Role of Na⁺ Interstitials and Dopants in Enhancing the Na⁺ Conductivity of the Cubic Na₃PS₄ Superionic Conductor. Chemistry of Materials, 2015, 27, 8318-8325.	6.7	202
114	Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening. Journal of Physical Chemistry Letters, 2015, 6, 283-291.	4.6	276
115	Relating voltage and thermal safety in Li-ion battery cathodes: a high-throughput computational study. Physical Chemistry Chemical Physics, 2015, 17, 5942-5953.	2.8	44
116	Rational Composition Optimization of the Lithium-Rich Li₃OCl_{1â€“x}Br_x Anti-Perovskite Superionic Conductors. Chemistry of Materials, 2015, 27, 3749-3755.	6.7	130
117	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	3.0	150
118	Design principles for solid-state lithium superionic conductors. Nature Materials, 2015, 14, 1026-1031.	27.5	1,079
119	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
120	Direct visualization of the Jahnâ€“Teller effect coupled to Na ordering in Na5/8MnO2. Nature Materials, 2014, 13, 586-592.	27.5	237
121	Nanoscale Stabilization of Sodium Oxides: Implications for Naâ€“O₂ Batteries. Nano Letters, 2014, 14, 1016-1020.	9.1	162
122	Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations. Chemistry of Materials, 2014, 26, 5208-5214.	6.7	149
123	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. Computational Materials Science, 2013, 68, 314-319.	3.0	2,392
124	Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. APL Materials, 2013, 1, .	5.1	6,913
125	Effect of Rb and Ta Doping on the Ionic Conductivity and Stability of the Garnet Li_{7+2xâ€“y}(La_{3â€“x}Rb_x)(Zr_{2â€“y}Ta_y)(0 â‰¤ x â‰¤ 0.375, 0 â‰¤ y â‰¤ 1) Superionic Conductor: A First Principles Investigation. Chemistry of Materials, 2013, 25, 3048-3055.	6.7	185
126	A Facile Mechanism for Recharging Li₂O₂ in Liâ€“O₂ Batteries. Chemistry of Materials, 2013, 25, 3328-3336.	6.7	179

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127	Phase stability, electrochemical stability and ionic conductivity of the Li_{10Â±1}MP₂X₁₂(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.	30.8	545
128	First-principles study of iron oxyfluorides and lithiation of FeOF. Physical Review B, 2013, 87, .	3.2	52
129	Designing Multielectron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals. Chemistry of Materials, 2013, 25, 2064-2074.	6.7	72
130	Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project. , 2012, , .		8
131	Low hole polaron migration barrier in lithium peroxide. Physical Review B, 2012, 85, .	3.2	158
132	First-principles insights on the magnetism of cubic SrTi1â^'xCoxO3â^'Î´. Applied Physics Letters, 2012, 100, 252904.	3.3	25
133	A comparison of destabilization mechanisms of the layered NaxMO2 and LixMO2 compounds upon alkali de-intercalation. Physical Chemistry Chemical Physics, 2012, 14, 15571.	2.8	158
134	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, .	3.2	380
135	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
136	First Principles Study of the Li₁₀GeP₂S₁₂ Lithium Super Ionic Conductor Material. Chemistry of Materials, 2012, 24, 15-17.	6.7	600
137	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. Chemistry of Materials, 2011, 23, 2979-2986.	6.7	337
138	First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery. Physical Review B, 2011, 84, .	3.2	191
139	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
140	A high-throughput infrastructure for density functional theory calculations. Computational Materials Science, 2011, 50, 2295-2310.	3.0	787
141	Formation enthalpies by mixing GGA and GGA<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>U</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2011, 84, .	3.2	853
142	Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput ab Initio Calculations. Chemistry of Materials, 2011, 23, 3495-3508.	6.7	363
143	Voltage, stability and diffusion barrier differences between sodium-ion and lithium-ion intercalation materials. Energy and Environmental Science, 2011, 4, 3680.	30.8	1,236
144	Comparison of small polaron migration and phase separation in olivine LiMnPO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>and LiFePO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mro	3.2	128

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145	Recharging lithium battery research with first-principles methods. MRS Bulletin, 2011, 36, 185-191.	3.5	143
146	Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations. Electrochemistry Communications, 2010, 12, 427-430.	4.7	224
147	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
148	Hybrid density functional calculations of redox potentials and formation energies of transition metal compounds. Physical Review B, 2010, 82, .	3.2	298
149	Liâ^'Feâ^'Pâ^'O₂ Phase Diagram from First Principles Calculations. Chemistry of Materials, 2008, 20, 1798-1807.	6.7	621