Yifei Mo

List of Publications by Year
in descending order

87 papers	16,931 citations	41323 49 h-index	54882 84 g-index
94 all docs	94 docs citations	94 times ranked	11562 citing authors

#	Article	IF	Citations
1	Negating interfacial impedance in garnet-based solid-state Li metal batteries. Nature Materials, 2017, 16, 572-579.	13.3	1,583
2	Origin of Outstanding Stability in the Lithium Solid Electrolyte Materials: Insights from Thermodynamic Analyses Based on First-Principles Calculations. ACS Applied Materials & Interfaces, 2015, 7, 23685-23693.	4.0	1,314
3	Design principles for solid-state lithium superionic conductors. Nature Materials, 2015, 14, 1026-1031.	13.3	1,079
4	Friction laws at the nanoscale. Nature, 2009, 457, 1116-1119.	13.7	783
5	Electrochemical Stability of Li₁₀GeP₂S₁₂ and Li₇La₃Zr₂O₁₂ Solid Electrolytes. Advanced Energy Materials, 2016, 6, 1501590.	10.2	781
6	First principles study on electrochemical and chemical stability of solid electrolyteâ€“electrode interfaces in all-solid-state Li-ion batteries. Journal of Materials Chemistry A, 2016, 4, 3253-3266.	5.2	748
7	Garnet-Type Solid-State Electrolytes: Materials, Interfaces, and Batteries. Chemical Reviews, 2020, 120, 4257-4300.	23.0	655
8	Toward garnet electrolyteâ€“based Li metal batteries: An ultrathin, highly effective, artificial solid-state electrolyte/metallic Li interface. Science Advances, 2017, 3, e1601659.	4.7	647
9	First Principles Study of the Li₁₀GeP₂S₁₂ Lithium Super Ionic Conductor Material. Chemistry of Materials, 2012, 24, 15-17.	3.2	600
10	Origin of fast ion diffusion in super-ionic conductors. Nature Communications, 2017, 8, 15893.	5.8	570
11	Transition from Superlithiophobicity to Superlithiophilicity of Garnet Solid-State Electrolyte. Journal of the American Chemical Society, 2016, 138, 12258-12262.	6.6	548
12	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.	15.6	545
13	Reducing Interfacial Resistance between Garnetâ€Structured Solidâ€State Electrolyte and Liâ€Metal Anode by a Germanium Layer. Advanced Materials, 2017, 29, 1606042.	11.1	512
14	Design Strategies, Practical Considerations, and New Solution Processes of Sulfide Solid Electrolytes for Allâ€Solidâ€State Batteries. Advanced Energy Materials, 2018, 8, 1800035.	10.2	410
15	A general method to synthesize and sinter bulk ceramics in seconds. Science, 2020, 368, 521-526.	6.0	357
16	Lithium Chlorides and Bromides as Promising Solidâ€State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. Angewandte Chemie - International Edition, 2019, 58, 8039-8043.	7.2	322
17	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	3.5	312
18	Computation-Accelerated Design of Materials and Interfaces for All-Solid-State Lithium-Ion Batteries. Joule, 2018, 2, 2016-2046.	11.7	266

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19	Site-Occupation-Tuned Superionic Li_{<i>x</i>}ScCl_{3+<i>x</i>}Halide Solid Electrolytes for All-Solid-State Batteries. Journal of the American Chemical Society, 2020, 142, 7012-7022.	6.6	260
20	Statistical variances of diffusional properties from ab initio molecular dynamics simulations. Npj Computational Materials, 2018, 4, .	3.5	240
21	Liquid phase therapy to solid electrolyteâ€“electrode interface in solid-state Li metal batteries: A review. Energy Storage Materials, 2020, 24, 75-84.	9.5	199
22	Lithiumâ€“Graphite Paste: An Interface Compatible Anode for Solidâ€State Batteries. Advanced Materials, 2019, 31, e1807243.	11.1	197
23	The Thermal Stability of Lithium Solid Electrolytes with Metallic Lithium. Joule, 2020, 4, 812-821.	11.7	197
24	First-principles study of the oxygen evolution reaction of lithium peroxide in the lithium-air battery. Physical Review B, 2011, 84, .	1.1	191
25	Effect of Rb and Ta Doping on the Ionic Conductivity and Stability of the Garnet Li_{7+2<i>x</i>â€“<i>y</i>}(La_{3â€“<i>x</i>}Rb_{<i>x</i>})(Zr_{2â€“<i>y</i>}Ta<sub><i>y< (0 â‰ <i>x</i> â‰ 0.375, 0 â‰ <i>y</i> â‰ 1) Superionic Conductor: A First Principles Investigation. Chemistry of Materials, 2013, 25, 3048-3055.	3.2	185
26	Strategies Based on Nitride Materials Chemistry to Stabilize Li Metal Anode. Advanced Science, 2017, 4, 1600517.	5.6	185
27	A Facile Mechanism for Recharging Li₂O₂ in Liâ€“O₂ Batteries. Chemistry of Materials, 2013, 25, 3328-3336.	3.2	179
28	Nanoscale Stabilization of Sodium Oxides: Implications for Naâ€“O₂ Batteries. Nano Letters, 2014, 14, 1016-1020.	4.5	162
29	Visualizing non-equilibrium lithiation of spinel oxide via in situ transmission electron microscopy. Nature Communications, 2016, 7, 11441.	5.8	162
30	Low hole polaron migration barrier in lithium peroxide. Physical Review B, 2012, 85, .	1.1	158
31	Denary oxide nanoparticles as highly stable catalysts for methane combustion. Nature Catalysis, 2021, 4, 62-70.	16.1	153
32	Unsupervised discovery of solid-state lithium ion conductors. Nature Communications, 2019, 10, 5260.	5.8	150
33	Insights into Diffusion Mechanisms in P2 Layered Oxide Materials by First-Principles Calculations. Chemistry of Materials, 2014, 26, 5208-5214.	3.2	149
34	Classical and Emerging Characterization Techniques for Investigation of Ion Transport Mechanisms in Crystalline Fast Ionic Conductors. Chemical Reviews, 2020, 120, 5954-6008.	23.0	140
35	Computational Studies of Electrode Materials in Sodiumâ€Ion Batteries. Advanced Energy Materials, 2018, 8, 1702998.	10.2	137
36	High energy-density and reversibility of iron fluoride cathode enabled via an intercalation-extrusion reaction. Nature Communications, 2018, 9, 2324.	5.8	136

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37	Sodiation Kinetics of Metal Oxide Conversion Electrodes: A Comparative Study with Lithiation. Nano Letters, 2015, 15, 5755-5763.	4.5	122
38	Materials Design Principles for Airâ€Stable Lithium/Sodium Solid Electrolytes. Angewandte Chemie - International Edition, 2020, 59, 17472-17476.	7.2	120
39	Stable Thiophosphate-Based All-Solid-State Lithium Batteries through Conformally Interfacial Nanocoating. Nano Letters, 2020, 20, 1483-1490.	4.5	112
40	Emerging Halide Superionic Conductors for All-Solid-State Batteries: Design, Synthesis, and Practical Applications. ACS Energy Letters, 2022, 7, 1776-1805.	8.8	106
41	Accelerated materials design of Na_{0.5}Bi_{0.5}TiO₃ oxygen ionic conductors based on first principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 18035-18044.	1.3	104
42	Crystal Structural Framework of Lithium Superâ€Ionic Conductors. Advanced Energy Materials, 2019, 9, 1902078.	10.2	93
43	Roughness picture of friction in dry nanoscale contacts. Physical Review B, 2010, 81, .	1.1	79
44	Computational studies of solid-state alkali conduction in rechargeable alkali-ion batteries. NPG Asia Materials, 2016, 8, e254-e254.	3.8	73
45	Stabilizing the Garnet Solid-Electrolyte/Polysulfide Interface in Liâ€“S Batteries. Chemistry of Materials, 2017, 29, 8037-8041.	3.2	73
46	Solid-State Chemistries Stable with High-Energy Cathodes for Lithium-Ion Batteries. ACS Energy Letters, 2019, 4, 2444-2451.	8.8	65
47	Advanced Highâ€Voltage Allâ€Solidâ€State Liâ€Ion Batteries Enabled by a Dualâ€Halogen Solid Electrolyte. Advanced Energy Materials, 2021, 11, 2100836.	10.2	64
48	Tailoring the Cation Lattice for Chloride Lithiumâ€Ion Conductors. Advanced Energy Materials, 2020, 10, 2002356.	10.2	56
49	Kinetic Phase Evolution of Spinel Cobalt Oxide during Lithiation. ACS Nano, 2016, 10, 9577-9585.	7.3	54
50	Interfacial Atomistic Mechanisms of Lithium Metal Stripping and Plating in Solidâ€State Batteries. Advanced Materials, 2021, 33, e2008081.	11.1	53
51	Multi-principal elemental intermetallic nanoparticles synthesized via a disorder-to-order transition. Science Advances, 2022, 8, eabm4322.	4.7	49
52	Simultaneous enhancement of toughness, ductility, and strength of nanocrystalline ceramics at high strain-rates. Applied Physics Letters, 2007, 90, 181926.	1.5	47
53	Elucidating Interfacial Stability between Lithium Metal Anode and Li Phosphorus Oxynitride via <i>In Situ</i> Electron Microscopy. Nano Letters, 2021, 21, 151-157.	4.5	36
54	Computationâ€Guided Design of LiTaSiO₅, a New Lithium Ionic Conductor with Sphene Structure. Advanced Energy Materials, 2019, 9, 1803821.	10.2	35

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55	Single-atom-layer traps in a solid electrolyte for lithium batteries. Nature Communications, 2020, 11, 1828.	5.8	35
56	Computation-guided discovery of coating materials to stabilize the interface between lithium garnet solid electrolyte and high-energy cathodes for all-solid-state lithium batteries. Energy Storage Materials, 2021, 41, 571-580.	9.5	31
57	Lithium Chlorides and Bromides as Promising Solidâ€State Chemistries for Fast Ion Conductors with Good Electrochemical Stability. Angewandte Chemie, 2019, 131, 8123-8127.	1.6	27
58	First-Principles Study of Oxyhydride Hâ€" Ion Conductors: Toward Facile Anion Conduction in Oxide-Based Materials. ACS Applied Energy Materials, 2018, 1, 1626-1634.	2.5	26
59	Origin of the isotope effect on solid friction. Physical Review B, 2009, 80, .	1.1	24
60	Interfacial Defect of Lithium Metal in Solidâ€State Batteries. Angewandte Chemie - International Edition, 2021, 60, 21494-21501.	7.2	20
61	First-Principles Computational Design and Discovery of Novel Double-Perovskite Proton Conductors. Chemistry of Materials, 2021, 33, 8278-8288.	3.2	19
62	A Computational Study of Fast Proton Diffusion in Brownmillerite Sr₂Co₂O₅. Chemistry of Materials, 2020, 32, 5028-5035.	3.2	17
63	Guiding Synthesis of Polymorphs of Materials Using Nanometric Phase Diagrams. Journal of the American Chemical Society, 2018, 140, 17290-17296.	6.6	15
64	Lithium ion storage in lithium titanium germanate. Nano Energy, 2019, 66, 104094.	8.2	15
65	Computationâ€Guided Synthesis of New Garnetâ€Type Solidâ€State Electrolytes via an Ultrafast Sintering Technique. Advanced Materials, 2020, 32, e2005059.	11.1	15
66	AlCl₃-Dosed Si(100)-2 Ã— 1: Adsorbates, Chlorinated Al Chains, and Incorporated Al. Journal of Physical Chemistry C, 2021, 125, 11336-11347.	1.5	14
67	Materials Design Principles for Airâ€Stable Lithium/Sodium Solid Electrolytes. Angewandte Chemie, 2020, 132, 17625-17629.	1.6	13
68	Strength of ultrananocrystalline diamond controlled by friction of buried interfaces. Journal Physics D: Applied Physics, 2011, 44, 405401.	1.3	12
69	First principles hybrid functional study of small polarons in doped SrCeO3 perovskite: towards computation design of materials with tailored polaron. Ionics, 2018, 24, 1139-1151.	1.2	12
70	Li⁺ Diffusion in Amorphous and Crystalline Al₂O₃ for Battery Electrode Coatings. Chemistry of Materials, 2021, 33, 7795-7804.	3.2	12
71	Can Substitutions Affect the Oxidative Stability of Lithium Argyrodite Solid Electrolytes?. ACS Applied Energy Materials, 2022, 5, 2045-2053.	2.5	11
72	Li₁₅P₄S₁₆Cl₃, a Lithium Chlorothiophosphate as a Solid-State Ionic Conductor. Inorganic Chemistry, 2020, 59, 226-234.	1.9	9

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73	First-Principles Computational Design and Discovery of Solid-Oxide Proton Conductors. Chemistry of Materials, 2022, 34, 5938-5948.	3.2	8
74	Single hot contacts. Nature Materials, 2013, 12, 9-11.	13.3	7
75	Interfacial Defect of Lithium Metal in Solidâ€State Batteries. Angewandte Chemie, 2021, 133, 21664-21671.	1.6	7
76	Postâ€lithium battery materials and technology. EcoMat, 2020, 2, e12048.	6.8	6
77	A Solid with Liquid-like Diffusion: A Unique Superionic Conductor. CheM, 2019, 5, 2289-2290.	5.8	5
78	Contrasting Reaction Modality between Electrochemical Sodiation and Lithiation in NiO Conversion Electrode Materials. Microscopy and Microanalysis, 2015, 21, 325-326.	0.2	2
79	Lithium Superâ€Ionic Conductors: Crystal Structural Framework of Lithium Superâ€Ionic Conductors (Adv. Energy Mater. 43/2019). Advanced Energy Materials, 2019, 9, 1970169.	10.2	2
80	Dopant precursor adsorption into single-dimer windows: Towards guided self-assembly of dopant arrays on Si(100). Chemical Physics Letters, 2022, 787, 139258.	1.2	2
81	A Molecular Dynamics Simulation of High Strain-rate Deformation in Nanocrystalline Silicon Carbide. Materials Research Society Symposia Proceedings, 2007, 1021, 1.	0.1	0
82	Improving the Ionic Conductivity of Li15P4S16Cl3 By Doping. ECS Meeting Abstracts, 2019, , .	0.0	0
83	Ab Initio Computation Design for Fast Ionic Conductors. ECS Meeting Abstracts, 2019, , .	0.0	0
84	Computation-Guided Exploration for New-Chemistry Solid Electrolyte with Fast Ion Conduction and Good Electrochemical Stability. ECS Meeting Abstracts, 2019, , .	0.0	0
85	Discovery of Novel Oxides and Sulfides Solid State Ionic Conductors for All-Solid-State Li-Ion Batteries. ECS Meeting Abstracts, 2019, , .	0.0	0
86	Data-Driven Discovery of New Materials for Solid-State Batteries. ECS Meeting Abstracts, 2020, MA2020-02, 201-201.	0.0	0
87	(Invited) Solid-State Chemistries Stable with High-Energy Cathodes for Lithium-Ion Batteries. ECS Meeting Abstracts, 2020, MA2020-02, 870-870.	0.0	0