

Siqi Shi

List of Publications by Year in descending order

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Version: 2024-02-01

104
papers

6,997
citations

71102

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58581

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106
all docs

106
docs citations

106
times ranked

7957
citing authors

#	ARTICLE	IF	CITATIONS
1	High Ion Selectivity of Garnet Solid Electrolyte Enabling Separation of Metallic Lithium. Energy and Environmental Materials, 2023, 6, .	12.8	1
2	Computational insights into the ionic transport mechanism and interfacial stability of the Li ₂ OHCl solid-state electrolyte. Journal of Materiomics, 2022, 8, 59-67.	5.7	19
3	Interfacial nitrogen engineering of robust silicon/MXene anode toward high energy solid-state lithium-ion batteries. Journal of Energy Chemistry, 2022, 67, 727-735.	12.9	46
4	Protective and ion conductive: High-Rate Ni-Rich cathode with enhanced cyclic stability via One-Step bifunctional dual-layer coating. Chemical Engineering Journal, 2022, 431, 134031.	12.7	13
5	Threshold potentials for fast kinetics during mediated redox catalysis of insulators in Li ⁺ O ₂ and Li ⁺ S batteries. Nature Catalysis, 2022, 5, 193-201.	34.4	51
6	Mg ₂ SiO ₄ /Si-Coated Disproportionated SiO Composite Anodes with High Initial Coulombic Efficiency for Lithium Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 15337-15345.	8.0	18
7	Identifying Hidden Li ⁺ Si ⁺ O Phases for Lithium-Ion Batteries via First-Principle Thermodynamic Calculations. Energy and Environmental Materials, 2022, 5, 865-871.	12.8	7
8	Composite cathode materials for next-generation lithium fluorinated carbon primary batteries. Journal of Power Sources, 2022, 541, 231716.	7.8	18
9	Identifying Chemical Factors Affecting Reaction Kinetics in Li-air Battery via ab initio Calculations and Machine Learning. Energy Storage Materials, 2021, 35, 595-601.	18.0	40
10	A highly efficient and informative method to identify ion transport networks in fast ion conductors. Acta Materialia, 2021, 203, 116490.	7.9	32
11	Metallic VS ₂ /graphene heterostructure as an ultra-high rate and high-specific capacity anode material for Li/Na-ion batteries. Physical Chemistry Chemical Physics, 2021, 23, 18784-18793.	2.8	20
12	Perfluorinated organics regulating Li ₂ O ₂ formation and improving stability for Li ⁺ oxygen batteries. Chemical Communications, 2021, 57, 3030-3033.	4.1	6
13	Machine learning prediction of activation energy in cubic Li-argyrodites with hierarchically encoding crystal structure-based (HECS) descriptors. Science Bulletin, 2021, 66, 1401-1408.	9.0	40
14	Induction of planar Li growth with designed interphases for dendrite-free Li metal anodes. Energy Storage Materials, 2021, 39, 250-258.	18.0	44
15	Understanding the Structural Evolution and Storage Mechanism of NASICON-Structure Mg _{0.5} Ti ₂ (PO ₄) ₃ for Li-Ion and Na-Ion Batteries. ACS Sustainable Chemistry and Engineering, 2021, 9, 13414-13423.	6.7	5
16	Identifying descriptors for Li ⁺ conduction in cubic Li-argyrodites via hierarchically encoding crystal structure and inferring causality. Energy Storage Materials, 2021, 40, 386-393.	18.0	24
17	Identifying Migration Channels and Bottlenecks in Monoclinic NASICON-type Solid Electrolytes with Hierarchical Ion Transport Algorithms. Advanced Functional Materials, 2021, 31, 2107747.	14.9	33
18	Domain Aggregation and Associated Pore Growth in Lipid Membranes. ACS Nano, 2021, 15, 604-613.	14.6	3

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19	GCNs-Based Context-Aware Short Text Similarity Model. , 2021, , .		0
20	Towards prediction of ordered phases in rechargeable battery chemistry via groupâ€“subgroup transformation. Npj Computational Materials, 2021, 7, .	8.7	8
21	Interpretability Analysis Method Based on Path Decomposition for Cell-based Neural Architecture Search. , 2021, , .		0
22	Methods and Applications of Causal Reasoning in Medical Field. , 2021, , .		1
23	Interpretability Latent Space Method: Exploiting Shapley Representation to Explain Latent Space. , 2021, , .		0
24	Ab initio thermodynamic optimization of Ni-rich Niâ€“Coâ€“Mn oxide cathode coatings. Journal of Power Sources, 2020, 450, 227693.	7.8	15
25	High-Throughput Computational Screening of Li-Containing Fluorides for Battery Cathode Coatings. ACS Sustainable Chemistry and Engineering, 2020, 8, 948-957.	6.7	34
26	Application of phase-field method in rechargeable batteries. Npj Computational Materials, 2020, 6, .	8.7	52
27	Ultrastable All-Solid-State Sodium Rechargeable Batteries. ACS Energy Letters, 2020, 5, 2835-2841.	17.4	142
28	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. National Science Review, 2020, 7, 1768-1775.	9.5	43
29	High Quality Pyrazinoquinoxaline-Based Graphdiyne for Efficient Gradient Storage of Lithium Ions. Nano Letters, 2020, 20, 7333-7341.	9.1	39
30	High-throughput screening platform for solid electrolytes combining hierarchical ion-transport prediction algorithms. Scientific Data, 2020, 7, 151.	5.3	90
31	Relationships Between Na ⁺ Distribution, Concerted Migration, and Diffusion Properties in Rhombohedral NASICON. Advanced Energy Materials, 2020, 10, 2001486.	19.5	64
32	CAVD, towards better characterization of void space for ionic transport analysis. Scientific Data, 2020, 7, 153.	5.3	43
33	Enabling reversible phase transition on K ₅ /9Mn ₇ /9Ti ₂ /9O ₂ for high-performance potassium-ion batteries cathodes. Energy Storage Materials, 2020, 31, 20-26.	18.0	35
34	Europium-Doped Ceria Nanowires as Anode for Solid Oxide Fuel Cells. Frontiers in Chemistry, 2020, 8, 348.	3.6	11
35	EML webinar overview: Simulation-assisted discovery of membrane targeting nanomedicine. Extreme Mechanics Letters, 2020, 39, 100817.	4.1	4
36	Ultrasml Co ₃ O ₄ Nanoparticles Confined in P, N-Doped Carbon Matrices for High-Performance Supercapacitors. Journal of Physical Chemistry C, 2020, 124, 9225-9232.	3.1	25

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37	Machine learning assisted materials design and discovery for rechargeable batteries. <i>Energy Storage Materials</i> , 2020, 31, 434-450.	18.0	212
38	Water in salt/ionic liquid electrolyte for 2.8 V aqueous lithium-ion capacitor. <i>Science Bulletin</i> , 2020, 65, 1812-1822.	9.0	56
39	A Database of Ionic Transport Characteristics for Over 29 000 Inorganic Compounds. <i>Advanced Functional Materials</i> , 2020, 30, 2003087.	14.9	42
40	Uncovering the Potential of Mn-Site Activated NASICON Cathodes for Zn-Ion Batteries. <i>Advanced Materials</i> , 2020, 32, e1907526.	21.0	103
41	Multi-Layer Feature Selection Incorporating Weighted Score-Based Expert Knowledge toward Modeling Materials with Targeted Properties. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900215.	2.8	74
42	Mobile Ions in Composite Solids. <i>Chemical Reviews</i> , 2020, 120, 4169-4221.	47.7	193
43	Predicting creep rupture life of Ni-based single crystal superalloys using divide-and-conquer approach based machine learning. <i>Acta Materialia</i> , 2020, 195, 454-467.	7.9	113
44	Understanding the Li diffusion mechanism and positive effect of current collector volume expansion in anode free batteries*. <i>Chinese Physics B</i> , 2020, 29, 068202.	1.4	31
45	Brief overview of microscopic physical image of ion transport in electrolytes. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020, 69, 226601.	0.5	27
46	Optimization of Organic/Water Hybrid Electrolytes for High-Rate Carbon-Based Supercapacitor. <i>Advanced Functional Materials</i> , 2019, 29, 1904136.	14.9	102
47	Rationalizing the interphase stability of Li ₇ La ₃ Zr ₂ O ₁₂ via automated reaction screening and machine learning. <i>Journal of Materials Chemistry A</i> , 2019, 7, 19961-19969.	10.3	59
48	A moisture absorbing gel electrolyte enables aqueous and flexible supercapacitors operating at high temperatures. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20398-20404.	10.3	57
49	Predicting the onset temperature (T _g) of Ge-Se glass transition: a feature selection based two-stage support vector regression method. <i>Science Bulletin</i> , 2019, 64, 1195-1203.	9.0	41
50	A Highly Reversible Zn Anode with Intrinsically Safe Organic Electrolyte for Long-Cycle-Life Batteries. <i>Advanced Materials</i> , 2019, 31, e1900668.	21.0	259
51	Correlated Migration Invokes Higher Na ⁺ Ion Conductivity in NaSICON-Type Solid Electrolytes. <i>Advanced Energy Materials</i> , 2019, 9, 1902373.	19.5	162
52	Mosquito bite prevention through graphene barrier layers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 18304-18309.	7.1	14
53	Revisiting the ionic diffusion mechanism in Li ₃ PS ₄ via the joint usage of geometrical analysis and bond valence method. <i>Journal of Materiomics</i> , 2019, 5, 688-695.	5.7	34
54	A viscoelastic adhesive epicardial patch for treating myocardial infarction. <i>Nature Biomedical Engineering</i> , 2019, 3, 632-643.	22.5	156

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55	Epicardial prestrained confinement and residual stresses: a newly observed heart ventricle confinement interface. <i>Journal of the Royal Society Interface</i> , 2019, 16, 20190028.	3.4	10
56	A sodium perchlorate-based hybrid electrolyte with high salt-to-water molar ratio for safe 2.5â€V carbon-based supercapacitor. <i>Energy Storage Materials</i> , 2019, 23, 603-609.	18.0	102
57	The Origin of Electrochemical Actuation of MnO ₂ /Ni Bilayer Film Derived by Redox Pseudocapacitive Process. <i>Advanced Functional Materials</i> , 2019, 29, 1806778.	14.9	59
58	In Situ Formed Shields Enabling Li ₂ CO ₃ -Free Solid Electrolytes: A New Route to Uncover the Intrinsic Lithiophilicity of Garnet Electrolytes for Dendrite-Free Li-Metal Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 898-905.	8.0	147
59	Spontaneous Growth of 3D Framework Carbon from Sodium Citrate for High Energyâ€and Powerâ€Density and Longâ€Life Sodiumâ€Ion Hybrid Capacitors. <i>Advanced Energy Materials</i> , 2018, 8, 1702409.	19.5	221
60	Visualization of the Diffusion Pathway of Protons in (NH ₄) ₂ Si _{0.5} Ti _{0.5} P ₄ O ₁₃ as an Electrolyte for Intermediate-Temperature Fuel Cells. <i>Inorganic Chemistry</i> , 2018, 57, 676-680.	4.0	7
61	Screening polyethylene oxide-based composite polymer electrolytes via combining effective medium theory and Halpin-Tsai model. <i>Computational Materials Science</i> , 2018, 144, 338-344.	3.0	17
62	Sprinkling MnFe ₂ O ₄ quantum dots on nitrogen-doped graphene sheets: the formation mechanism and application for high-performance supercapacitor electrodes. <i>Journal of Materials Chemistry A</i> , 2018, 6, 9997-10007.	10.3	59
63	Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. <i>Npj Computational Materials</i> , 2018, 4, .	8.7	961
64	First-Principles Study of MoO ₃ /Graphene Composite as Cathode Material for High-Performance Lithium-Ion Batteries. <i>Applied Surface Science</i> , 2018, 433, 1083-1093.	6.1	27
65	The Influence Maximization Problem in the Network Under Node Personalized Characteristics. , 2018, , .		1
66	Rotational motion of polyanion versus volume effect associated with ionic conductivity of several solid electrolytes. <i>Rare Metals</i> , 2018, 37, 497-503.	7.1	36
67	Safe and high-rate supercapacitors based on an â€acetonitrile/water in saltâ€hybrid electrolyte. <i>Energy and Environmental Science</i> , 2018, 11, 3212-3219.	30.8	297
68	A combined DFT and experimental study on the nucleation mechanism of NiO nanodots on graphene. <i>Journal of Materials Chemistry A</i> , 2018, 6, 13717-13724.	10.3	17
69	An Î±-CrPO ₄ -type NaV ₃ (PO ₄) ₃ anode for sodium-ion batteries with excellent cycling stability and the exploration of sodium storage behavior. <i>Journal of Materials Chemistry A</i> , 2017, 5, 3839-3847.	10.3	24
70	Quantitative description on structureâ€property relationships of Li-ion battery materials for high-throughput computations. <i>Science and Technology of Advanced Materials</i> , 2017, 18, 134-146.	6.1	21
71	Low temperature fabrication of thermochromic VO ₂ thin films by low-pressure chemical vapor deposition. <i>RSC Advances</i> , 2017, 7, 10798-10805.	3.6	24
72	First-principles insight into the structural fundamental of super ionic conducting in NASICON MTi ₂ (PO ₄) ₃ (M = Li, Na) materials for rechargeable batteries. <i>Nano Energy</i> , 2017, 41, 626-633.	16.0	67

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73	Antisite occupation induced single anionic redox chemistry and structural stabilization of layered sodium chromium sulfide. <i>Nature Communications</i> , 2017, 8, 566.	12.8	81
74	Materials discovery and design using machine learning. <i>Journal of Materiomics</i> , 2017, 3, 159-177.	5.7	629
75	Estimation of adjacent substitution rate based on clustering algorithm and its application. , 2016, , .		0
76	First-principles study of the effect of oxygen vacancy and strain on the phase transition temperature of VO ₂ . <i>RSC Advances</i> , 2016, 6, 86872-86879.	3.6	32
77	Elastic Properties, Defect Thermodynamics, Electrochemical Window, Phase Stability, and Li ⁺ Mobility of Li ₃ PS ₄ : Insights from First-Principles Calculations. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 25229-25242.	8.0	114
78	Tuning the phase transition temperature, electrical and optical properties of VO ₂ by oxygen nonstoichiometry: insights from first-principles calculations. <i>RSC Advances</i> , 2016, 6, 73070-73082.	3.6	42
79	Lattice dynamics, thermodynamics and elastic properties of C22-Zr6FeSn2 from first-principles calculations. <i>Journal of Nuclear Materials</i> , 2016, 479, 461-469.	2.7	12
80	Cluster expansion method and its application in computational materials science. <i>Computational Materials Science</i> , 2016, 125, 243-254.	3.0	59
81	Enhanced coking tolerance of a MgO-modified Ni cermet anode for hydrocarbon fueled solid oxide fuel cells. <i>Journal of Materials Chemistry A</i> , 2016, 4, 18031-18036.	10.3	45
82	NaV3(PO4)3/C nanocomposite as novel anode material for Na-ion batteries with high stability. <i>Nano Energy</i> , 2016, 26, 382-391.	16.0	69
83	A Novel Small-Molecule Compound of Lithium Iodine and 3-Hydroxypropionitrile as a Solid-State Electrolyte for Lithium-Air Batteries. <i>Inorganic Chemistry</i> , 2016, 55, 6504-6510.	4.0	15
84	Sputtering Deposition of Sandwich-Structured V ₂ O ₅ /Metal (V), Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 312 Td Sensitive VO ₂ Thin Films with Selectivity of VO ₂ (B) and VO ₂ (M) Polymorph. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 7884-7890.	8.0	66
85	Lithium-ion transport in inorganic solid state electrolyte. <i>Chinese Physics B</i> , 2016, 25, 018211.	1.4	66
86	Experimental Study and Stabilization Mechanisms of Silica Nanoparticles Based Brine Mud with High Temperature Resistance for Horizontal Shale Gas Wells. <i>Journal of Nanomaterials</i> , 2015, 2015, 1-9.	2.7	14
87	Hydrogen-doping induced reduction in the phase transition temperature of VO ₂ : a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20998-21004.	2.8	47
88	Discrete Li-occupation versus pseudo-continuous Na-occupation and their relationship with structural change behaviors in Fe ₂ (MoO ₄) ₃ . <i>Scientific Reports</i> , 2015, 5, 8810.	3.3	42
89	Survivability-Aware Topology Evolution Model with Link and Node Deletion in Wireless Sensor Networks. <i>International Journal of Distributed Sensor Networks</i> , 2014, 10, 278629.	2.2	0
90	Prediction of soil moisture based on Extreme Learning Machine for an apple orchard. , 2014, , .		5

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91	Defect Thermodynamics and Diffusion Mechanisms in Li_2CO_3 and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 8579-8593.	3.1	228
92	The study of the agricultural product storage temperature and humidity control system. , 2013, , .		1
93	Information Gain with Weight Based Decision Tree for the Employment Forecasting of Undergraduates. , 2013, , .		7
94	A software engineering practice platform based on event ontology. , 2012, , .		1
95	Time-Based K-nearest Neighbor Collaborative Filtering. , 2012, , .		1
96	Direct Calculation of Li-Ion Transport in the Solid Electrolyte Interphase. Journal of the American Chemical Society, 2012, 134, 15476-15487.	13.7	524
97	User-Session-Based Test Cases Optimization Method Based on Agglomerate Hierarchy Clustering. , 2011, , .		8
98	Computational Grid Based Neural Network Ensemble Learning Platform and Its Application. , 2009, , .		2
99	Wrapper Feature Selection Optimized SVM Model for Demand Forecasting. , 2008, , .		14
100	Using Rough Reducts Based SVM Ensemble for SAR of the Ethofenprox Analogous of Pesticide. , 2008, , .		0
101	Support vector machine method for forecasting future strong earthquakes in Chinese mainland. Acta Seismologica Sinica, 2006, 19, 30-38.	0.2	2
102	Extraction of if-then rules from trained neural network and its application to earthquake prediction. , 2004, , .		9
103	Impulse force based ART network with GA optimization. , 2003, , .		4
104	Ensemble algorithm of neural networks and its application. , 0, , .		0