

# Siqi Shi

## List of Publications by Year in descending order

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104  
papers

6,997  
citations

71102

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82  
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106  
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106  
docs citations

106  
times ranked

7957  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. Npj Computational Materials, 2018, 4, .   | 8.7  | 961       |
| 2  | Materials discovery and design using machine learning. Journal of Materiomics, 2017, 3, 159-177.  | 5.7  | 629       |
| 3  | Direct Calculation of Li-Ion Transport in the Solid Electrolyte Interphase. Journal of the American Chemical Society, 2012, 134, 15476-15487.   | 13.7 | 524       |
| 4  | Safe and high-rate supercapacitors based on an "acetonitrile/water in salt" hybrid electrolyte. Energy and Environmental Science, 2018, 11, 3212-3219.  | 30.8 | 297       |
| 5  | A Highly Reversible Zn Anode with Intrinsically Safe Organic Electrolyte for Long-Cycle-Life Batteries. Advanced Materials, 2019, 31, e1900668.   | 21.0 | 259       |
| 6  | Defect Thermodynamics and Diffusion Mechanisms in $\text{Li}_2\text{CO}_3$ and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 8579-8593.  | 3.1  | 228       |
| 7  | Spontaneous Growth of 3D Framework Carbon from Sodium Citrate for High Energy-Density and Long-Life Sodium-Ion Hybrid Capacitors. Advanced Energy Materials, 2018, 8, 1702409.  | 19.5 | 221       |
| 8  | Machine learning assisted materials design and discovery for rechargeable batteries. Energy Storage Materials, 2020, 31, 434-450.   | 18.0 | 212       |
| 9  | Mobile Ions in Composite Solids. Chemical Reviews, 2020, 120, 4169-4221.  | 47.7 | 193       |
| 10 | Correlated Migration Invokes Higher $\text{Na}^+$ Ion Conductivity in NaSICON-Type Solid Electrolytes. Advanced Energy Materials, 2019, 9, 1902373.   | 19.5 | 162       |
| 11 | A viscoelastic adhesive epicardial patch for treating myocardial infarction. Nature Biomedical Engineering, 2019, 3, 632-643.   | 22.5 | 156       |
| 12 | In Situ Formed Shields Enabling $\text{Li}_2\text{CO}_3$ -Free Solid Electrolytes: A New Route to Uncover the Intrinsic Lithiophilicity of Garnet Electrolytes for Dendrite-Free Li-Metal Batteries. ACS Applied Materials & Interfaces, 2019, 11, 898-905. | 8.0  | 147       |
| 13 | Ultrastable All-Solid-State Sodium Rechargeable Batteries. ACS Energy Letters, 2020, 5, 2835-2841.  | 17.4 | 142       |
| 14 | Elastic Properties, Defect Thermodynamics, Electrochemical Window, Phase Stability, and $\text{Li}^+$ Mobility of $\text{Li}_3\text{PS}_4$ : Insights from First-Principles Calculations. ACS Applied Materials & Interfaces, 2016, 8, 25229-25242.         | 8.0  | 114       |
| 15 | Predicting creep rupture life of Ni-based single crystal superalloys using divide-and-conquer approach based machine learning. Acta Materialia, 2020, 195, 454-467.   | 7.9  | 113       |
| 16 | Uncovering the Potential of Mn-Site-Activated NASICON Cathodes for Zn-Ion Batteries. Advanced Materials, 2020, 32, e1907526.  | 21.0 | 103       |
| 17 | Optimization of Organic/Water Hybrid Electrolytes for High-Rate Carbon-Based Supercapacitor. Advanced Functional Materials, 2019, 29, 1904136.  | 14.9 | 102       |
| 18 | A sodium perchlorate-based hybrid electrolyte with high salt-to-water molar ratio for safe 2.5 V carbon-based supercapacitor. Energy Storage Materials, 2019, 23, 603-609.  | 18.0 | 102       |

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|----|--|------|-----------|
| 19 | High-throughput screening platform for solid electrolytes combining hierarchical ion-transport prediction algorithms. <i>Scientific Data</i> , 2020, 7, 151.   | 5.3  | 90        |
| 20 | 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        |
| 21 | 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        |
| 22 | NaV <sub>3</sub> (PO <sub>4</sub> ) <sub>3</sub> /C nanocomposite as novel anode material for Na-ion batteries with high stability. <i>Nano Energy</i> , 2016, 26, 382-391.  | 16.0 | 69        |
| 23 | First-principles insight into the structural fundamental of super ionic conducting in NASICON MTi <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> (M = Li, Na) materials for rechargeable batteries. <i>Nano Energy</i> , 2017, 41, 626-633.  | 16.0 | 67        |
| 24 | Sputtering Deposition of Sandwich-Structured V <sub>2</sub> O <sub>5</sub> /Metal (V,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 552 Td Sensitive VO <sub>2</sub> Thin Films with Selectivity of VO <sub>2</sub> (B) and VO <sub>2</sub> (M) Polymorph. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 7884-7890. | 8.0  | 66        |
| 25 | Lithium-ion transport in inorganic solid state electrolyte. <i>Chinese Physics B</i> , 2016, 25, 018211.   | 1.4  | 66        |
| 26 | Relationships Between Na <sup>+</sup> Distribution, Concerted Migration, and Diffusion Properties in Rhombohedral NASICON. <i>Advanced Energy Materials</i> , 2020, 10, 2001486.   | 19.5 | 64        |
| 27 | Cluster expansion method and its application in computational materials science. <i>Computational Materials Science</i> , 2016, 125, 243-254.  | 3.0  | 59        |
| 28 | Sprinkling MnFe <sub>2</sub> O <sub>4</sub> 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        |
| 29 | Rationalizing the interphase stability of Li <sup>+</sup> doped-Li <sub>7</sub> La <sub>3</sub> Zr <sub>2</sub> O <sub>12</sub> via automated reaction screening and machine learning. <i>Journal of Materials Chemistry A</i> , 2019, 7, 19961-19969.   | 10.3 | 59        |
| 30 | The Origin of Electrochemical Actuation of MnO <sub>2</sub> /Ni Bilayer Film Derived by Redox Pseudocapacitive Process. <i>Advanced Functional Materials</i> , 2019, 29, 1806778.  | 14.9 | 59        |
| 31 | 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        |
| 32 | Water in salt/ionic liquid electrolyte for 2.8V aqueous lithium-ion capacitor. <i>Science Bulletin</i> , 2020, 65, 1812-1822.  | 9.0  | 56        |
| 33 | Application of phase-field method in rechargeable batteries. <i>Npj Computational Materials</i> , 2020, 6, .   | 8.7  | 52        |
| 34 | Threshold potentials for fast kinetics during mediated redox catalysis of insulators in Li <sup>+</sup> O <sub>2</sub> and Li <sup>+</sup> S batteries. <i>Nature Catalysis</i> , 2022, 5, 193-201.  | 34.4 | 51        |
| 35 | Hydrogen-doping induced reduction in the phase transition temperature of VO <sub>2</sub> : a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20998-21004.   | 2.8  | 47        |
| 36 | Interfacial nitrogen engineering of robust silicon/MXene anode toward high energy solid-state lithium-ion batteries. <i>Journal of Energy Chemistry</i> , 2022, 67, 727-735.   | 12.9 | 46        |

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|----|--|------|-----------|
| 37 | 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        |
| 38 | Induction of planar Li growth with designed interphases for dendrite-free Li metal anodes. <i>Energy Storage Materials</i> , 2021, 39, 250-258.  | 18.0 | 44        |
| 39 | Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. <i>National Science Review</i> , 2020, 7, 1768-1775.   | 9.5  | 43        |
| 40 | CAVD, towards better characterization of void space for ionic transport analysis. <i>Scientific Data</i> , 2020, 7, 153.   | 5.3  | 43        |
| 41 | Discrete Li-occupation versus pseudo-continuous Na-occupation and their relationship with structural change behaviors in Fe <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub> . <i>Scientific Reports</i> , 2015, 5, 8810. | 3.3  | 42        |
| 42 | Tuning the phase transition temperature, electrical and optical properties of VO <sub>2</sub> by oxygen nonstoichiometry: insights from first-principles calculations. <i>RSC Advances</i> , 2016, 6, 73070-73082.     | 3.6  | 42        |
| 43 | A Database of Ionic Transport Characteristics for Over 29 000 Inorganic Compounds. <i>Advanced Functional Materials</i> , 2020, 30, 2003087.   | 14.9 | 42        |
| 44 | Predicting the onset temperature (T <sub>g</sub> ) of Ge Se <sup>1</sup> glass transition: a feature selection based two-stage support vector regression method. <i>Science Bulletin</i> , 2019, 64, 1195-1203.        | 9.0  | 41        |
| 45 | Identifying Chemical Factors Affecting Reaction Kinetics in Li-air Battery via ab initio Calculations and Machine Learning. <i>Energy Storage Materials</i> , 2021, 35, 595-601.                                       | 18.0 | 40        |
| 46 | Machine learning prediction of activation energy in cubic Li-argyrodites with hierarchically encoding crystal structure-based (HECS) descriptors. <i>Science Bulletin</i> , 2021, 66, 1401-1408.                       | 9.0  | 40        |
| 47 | High Quality Pyrazinoquinoxaline-Based Graphdiyne for Efficient Gradient Storage of Lithium Ions. <i>Nano Letters</i> , 2020, 20, 7333-7341.   | 9.1  | 39        |
| 48 | 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        |
| 49 | Enabling reversible phase transition on K <sub>5</sub> /9Mn <sub>7</sub> /9Ti <sub>2</sub> /9O <sub>2</sub> for high-performance potassium-ion batteries cathodes. <i>Energy Storage Materials</i> , 2020, 31, 20-26.  | 18.0 | 35        |
| 50 | Revisiting the ionic diffusion mechanism in Li <sub>3</sub> PS <sub>4</sub> via the joint usage of geometrical analysis and bond valence method. <i>Journal of Materiomics</i> , 2019, 5, 688-695.                     | 5.7  | 34        |
| 51 | High-Throughput Computational Screening of Li-Containing Fluorides for Battery Cathode Coatings. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 948-957.  | 6.7  | 34        |
| 52 | Identifying Migration Channels and Bottlenecks in Monoclinic NASICON-type Solid Electrolytes with Hierarchical Ion Transport Algorithms. <i>Advanced Functional Materials</i> , 2021, 31, 2107747.                     | 14.9 | 33        |
| 53 | First-principles study of the effect of oxygen vacancy and strain on the phase transition temperature of VO <sub>2</sub> . <i>RSC Advances</i> , 2016, 6, 86872-86879.   | 3.6  | 32        |
| 54 | A highly efficient and informative method to identify ion transport networks in fast ion conductors. <i>Acta Materialia</i> , 2021, 203, 116490.   | 7.9  | 32        |

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|----|--|------|-----------|
| 55 | Understanding the Li diffusion mechanism and positive effect of current collector volume expansion in anode free batteries*. Chinese Physics B, 2020, 29, 068202.  | 1.4  | 31        |
| 56 | First-Principles Study of MoO <sub>3</sub> /Graphene Composite as Cathode Material for High-Performance Lithium-Ion Batteries. Applied Surface Science, 2018, 433, 1083-1093.  | 6.1  | 27        |
| 57 | Brief overview of microscopic physical image of ion transport in electrolytes. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 226601.  | 0.5  | 27        |
| 58 | Ultrasmall Co <sub>3</sub> O <sub>4</sub> Nanoparticles Confined in P, N-Doped Carbon Matrices for High-Performance Supercapacitors. Journal of Physical Chemistry C, 2020, 124, 9225-9232.                                  | 3.1  | 25        |
| 59 | An $\text{CrPO}_4$ -type $\text{NaV}_3(\text{PO}_4)_3$ anode for sodium-ion batteries with excellent cycling stability and the exploration of sodium storage behavior. Journal of Materials Chemistry A, 2017, 5, 3839-3847. | 10.3 | 24        |
| 60 | Low temperature fabrication of thermochromic VO <sub>2</sub> thin films by low-pressure chemical vapor deposition. RSC Advances, 2017, 7, 10798-10805.   | 3.6  | 24        |
| 61 | Identifying descriptors for Li <sup>+</sup> conduction in cubic Li-argyrodites via hierarchically encoding crystal structure and inferring causality. Energy Storage Materials, 2021, 40, 386-393.                           | 18.0 | 24        |
| 62 | Quantitative description on structure–property relationships of Li-ion battery materials for high-throughput computations. Science and Technology of Advanced Materials, 2017, 18, 134-146.                                  | 6.1  | 21        |
| 63 | Metallic VS <sub>2</sub> /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        |
| 64 | Computational insights into the ionic transport mechanism and interfacial stability of the Li <sub>2</sub> OHCl solid-state electrolyte. Journal of Materiomics, 2022, 8, 59-67.   | 5.7  | 19        |
| 65 | Mg <sub>2</sub> SiO <sub>4</sub> /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        |
| 66 | Composite cathode materials for next-generation lithium fluorinated carbon primary batteries. Journal of Power Sources, 2022, 541, 231716.   | 7.8  | 18        |
| 67 | Screening polyethylene oxide-based composite polymer electrolytes via combining effective medium theory and Halpin-Tsai model. Computational Materials Science, 2018, 144, 338-344.  | 3.0  | 17        |
| 68 | A combined DFT and experimental study on the nucleation mechanism of NiO nanodots on graphene. Journal of Materials Chemistry A, 2018, 6, 13717-13724.   | 10.3 | 17        |
| 69 | A Novel Small-Molecule Compound of Lithium Iodine and 3-Hydroxypropionitrile as a Solid-State Electrolyte for Lithium–Air Batteries. Inorganic Chemistry, 2016, 55, 6504-6510.   | 4.0  | 15        |
| 70 | Ab initio thermodynamic optimization of Ni-rich Ni–Co–Mn oxide cathode coatings. Journal of Power Sources, 2020, 450, 227693.  | 7.8  | 15        |
| 71 | Wrapper Feature Selection Optimized SVM Model for Demand Forecasting. , 2008, , .  |      | 14        |
| 72 | Experimental Study and Stabilization Mechanisms of Silica Nanoparticles Based Brine Mud with High Temperature Resistance for Horizontal Shale Gas Wells. Journal of Nanomaterials, 2015, 2015, 1-9.                          | 2.7  | 14        |

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|----|--|------|-----------|
| 73 | Mosquito bite prevention through graphene barrier layers. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18304-18309.   | 7.1  | 14        |
| 74 | 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        |
| 75 | Lattice dynamics, thermodynamics and elastic properties of C22-Zr6FeSn2 from first-principles calculations. Journal of Nuclear Materials, 2016, 479, 461-469.  | 2.7  | 12        |
| 76 | Europium-Doped Ceria Nanowires as Anode for Solid Oxide Fuel Cells. Frontiers in Chemistry, 2020, 8, 348.  | 3.6  | 11        |
| 77 | Epicardial prestrained confinement and residual stresses: a newly observed heart ventricle confinement interface. Journal of the Royal Society Interface, 2019, 16, 20190028.  | 3.4  | 10        |
| 78 | Extraction of if-then rules from trained neural network and its application to earthquake prediction. , 2004, , .  |      | 9         |
| 79 | User-Session-Based Test Cases Optimization Method Based on Agglutinate Hierarchy Clustering. , 2011, , .   |      | 8         |
| 80 | Towards prediction of ordered phases in rechargeable battery chemistry via groupâ€“subgroup transformation. Npj Computational Materials, 2021, 7, .  | 8.7  | 8         |
| 81 | Information Gain with Weight Based Decision Tree for the Employment Forecasting of Undergraduates. , 2013, , .   |      | 7         |
| 82 | Visualization of the Diffusion Pathway of Protons in (NH4)2Si0.5Ti0.5P4O13 as an Electrolyte for Intermediate-Temperature Fuel Cells. Inorganic Chemistry, 2018, 57, 676-680.  | 4.0  | 7         |
| 83 | Identifying Hidden Liâ€“Siâ€“O Phases for Lithiumâ€“Ion Batteries via Firstâ€“Principle Thermodynamic Calculations. Energy and Environmental Materials, 2022, 5, 865-871.  | 12.8 | 7         |
| 84 | Perfluorinated organics regulating Li<sub>2</sub>O<sub>2</sub> formation and improving stability for Liâ€“oxygen batteries. Chemical Communications, 2021, 57, 3030-3033.  | 4.1  | 6         |
| 85 | Prediction of soil moisture based on Extreme Learning Machine for an apple orchard. , 2014, , .  |      | 5         |
| 86 | Understanding the Structural Evolution and Storage Mechanism of NASICON-Structure Mg<sub>0.5</sub>Ti<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> for Li-Ion and Na-Ion Batteries. ACS Sustainable Chemistry and Engineering, 2021, 9, 13414-13423. | 6.7  | 5         |
| 87 | Impulse force based ART network with GA optimization. , 2003, , .  |      | 4         |
| 88 | EML webinar overview: Simulation-assisted discovery of membrane targeting nanomedicine. Extreme Mechanics Letters, 2020, 39, 100817.   | 4.1  | 4         |
| 89 | Domain Aggregation and Associated Pore Growth in Lipid Membranes. ACS Nano, 2021, 15, 604-613.   | 14.6 | 3         |
| 90 | Support vector machine method for forecasting future strong earthquakes in Chinese mainland. Acta Seismologica Sinica, 2006, 19, 30-38.  | 0.2  | 2         |

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|-----|---|------|-----------|
| 91  | Computational Grid Based Neural Network Ensemble Learning Platform and Its Application. , 2009, , .   |      | 2         |
| 92  | A software engineering practice platform based on event ontology. , 2012, , .   |      | 1         |
| 93  | Time-Based K-nearest Neighbor Collaborative Filtering. , 2012, , .  |      | 1         |
| 94  | The study of the agricultural product storage temperature and humidity control system. , 2013, , .  |      | 1         |
| 95  | The Influence Maximization Problem in the Network Under Node Personalized Characteristics. , 2018, , .  |      | 1         |
| 96  | Methods and Applications of Causal Reasoning in Medical Field. , 2021, , .  |      | 1         |
| 97  | High Ion-Selectivity of Garnet Solid Electrolyte Enabling Separation of Metallic Lithium. Energy and Environmental Materials, 2023, 6, .                                      | 12.8 | 1         |
| 98  | Ensemble algorithm of neural networks and its application. , 0, , .   |      | 0         |
| 99  | Using Rough Reducts Based SVM Ensemble for SAR of the Ethofenprox Analogous of Pesticide. , 2008, , .   |      | 0         |
| 100 | Survivability-Aware Topology Evolution Model with Link and Node Deletion in Wireless Sensor Networks. International Journal of Distributed Sensor Networks, 2014, 10, 278629. | 2.2  | 0         |
| 101 | Estimation of adjacent substitution rate based on clustering algorithm and its application. , 2016, , .   |      | 0         |
| 102 | GCNs-Based Context-Aware Short Text Similarity Model. , 2021, , .   |      | 0         |
| 103 | Interpretability Analysis Method Based on Path Decomposition for Cell-based Neural Architecture Search. , 2021, , .   |      | 0         |
| 104 | Interpretability Latent Space Method: Exploiting Shapley Representation to Explain Latent Space. , 2021, , .  |      | 0         |