Zhong-Heng Fu

List of Publications by Year
in descending order

39 papers	2,945 citations	304368 22 h-index	301761 39 g-index
39 all docs	39 docs citations	39 times ranked	4113 citing authors

#	Article	IF	Citations
1	Review on the lithium transport mechanism in solidâ€state battery materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	11
2	The chemical origin of temperature-dependent lithium-ion concerted diffusion in sulfide solid electrolyte Li10GeP2S12. Journal of Energy Chemistry, 2022, 70, 59-66.	7.1	22
3	A review on theoretical models for lithiumâ€“sulfur battery cathodes. InformaÄnÃ-MateriÃ¡ly, 2022, 4, .	8.5	143
4	Applying Classical, Ab Initio, and Machine-Learning Molecular Dynamics Simulations to the Liquid Electrolyte for Rechargeable Batteries. Chemical Reviews, 2022, 122, 10970-11021.	23.0	138
5	Anodeâ€Free Solidâ€State Lithium Batteries: A Review. Advanced Energy Materials, 2022, 12, .	10.2	81
6	The Origin of Fast Lithiumâ€Ion Transport in the Inorganic Solid Electrolyte Interphase on Lithium Metal Anodes. Small Structures, 2022, 3, .	6.9	42
7	Two-Dimensional Carbonitride MXenes as an Efficient Electrocatalyst for Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 4477-4488.	1.5	13
8	Stress Regulation on Atomic Bonding and Ionic Diffusivity: Mechanochemical Effects in Sulfide Solid Electrolytes. Energy & Fuels, 2021, 35, 10210-10218.	2.5	22
9	Giant heterogeneous magnetostriction induced by charge accumulation-mediated nanoinclusion formation in dual-phase nanostructured systems. Acta Materialia, 2021, 213, 116975.	3.8	20
10	An Atomic Insight into the Chemical Origin and Variation of the Dielectric Constant in Liquid Electrolytes. Angewandte Chemie, 2021, 133, 21643-21648.	1.6	9
11	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
12	Single Atomâ€Modified Hybrid Transition Metal Carbides as Efficient Hydrogen Evolution Reaction Catalysts. Advanced Functional Materials, 2021, 31, 2104285.	7.8	42
13	An Atomic Insight into the Chemical Origin and Variation of the Dielectric Constant in Liquid Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 21473-21478.	7.2	74
14	The carrier transition from Li atoms to Li vacancies in solid-state lithium alloy anodes. Science Advances, 2021, 7, eabi5520.	4.7	110
15	Magnetocrystalline anisotropy regulations in bulk L10-MnGa alloys by tailoring the tetragonal lattice parameter c: Selectively alloying Al and C atoms. Journal of Alloys and Compounds, 2021, 881, 160646.	2.8	2
16	Single-atom-Ni-decorated, nitrogen-doped carbon layers for efficient electrocatalytic CO2 reduction reaction. Electrochemistry Communications, 2020, 116, 106758.	2.3	31
17	Designing Flexible Quantum Spin Hall Insulators through 2D Ordered Hybrid Transition-Metal Carbides. Journal of Physical Chemistry C, 2019, 123, 20664-20674.	1.5	4
18	High-performance microwave absorption of hierarchical graphene-based and MWCNT-based full-carbon nanostructures. Applied Surface Science, 2019, 493, 541-550.	3.1	18

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19	Designing ultrastrong 5d transition metal diborides with excellent stability for harsh service environments. Physical Chemistry Chemical Physics, 2019, 21, 16095-16107.	1.3	7
20	First-principles design of strong solids: Approaches and applications. Physics Reports, 2019, 826, 1-49.	10.3	31
21	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. Chemical Reviews, 2019, 119, 11980-12031.	23.0	242
22	Uniaxial magnetocrystalline anisotropy of tetragonal Mn Ga100â^' (50â€¯â‰¤â€¯xâ€¯â‰¤â€¯75) alloys. Journal of Magnetism and Magnetic Materials, 2019, 489, 165308.	1.0	8
23	ADAIS: Automatic Derivation of Anisotropic Ideal Strength via high-throughput first-principles computations. Computer Physics Communications, 2019, 238, 244-253.	3.0	24
24	Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition-Metal Carbides. Journal of Physical Chemistry C, 2018, 122, 4710-4722.	1.5	28
25	Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of Ti₂CO₂ and Mo₂CO₂. Physical Chemistry Chemical Physics, 2018, 20, 14608-14618.	1.3	8
26	High-throughput theoretical optimization of the hydrogen evolution reaction on MXenes by transition metal modification. Journal of Materials Chemistry A, 2018, 6, 4271-4278.	5.2	198
27	Stabilization of Ï„-phase in carbon-doped MnAl magnetic alloys. Journal of Alloys and Compounds, 2018, 755, 257-264.	2.8	36
28	A synergetic stabilization and strengthening strategy for two-dimensional ordered hybrid transition metal carbides. Physical Chemistry Chemical Physics, 2018, 20, 29684-29692.	1.3	9
29	Surface Electrochemical Stability and Strainâ€Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. Advanced Functional Materials, 2018, 28, 1804867.	7.8	33
30	Highly Air-Stable Carbon-Based Î±-CsPbI₃ Perovskite Solar Cells with a Broadened Optical Spectrum. ACS Energy Letters, 2018, 3, 1824-1831.	8.8	235
31	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. Carbon, 2018, 137, 156-164.	5.4	22
32	Theoretical Investigation of 2D Layered Materials as Protective Films for Lithium and Sodium Metal Anodes. Advanced Energy Materials, 2017, 7, 1602528.	10.2	196
33	Designing flexible 2D transition metal carbides with strain-controllable lithium storage. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11082-E11091.	3.3	51
34	Stacking stability and sliding mechanism in weakly bonded 2D transition metal carbides by van der Waals force. RSC Advances, 2017, 7, 55912-55919.	1.7	53
35	Indirect-Direct Band Transformation of Few-Layer BiOCl under Biaxial Strain. Journal of Physical Chemistry C, 2016, 120, 8589-8594.	1.5	29
36	Domain-dependent electronic structure and optical absorption property in hybrid organicâ€“inorganic perovskite. Physical Chemistry Chemical Physics, 2016, 18, 27358-27365.	1.3	10

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37	Pinning effect of reactive elements on adhesion energy and adhesive strength of incoherent Al₂O₃/NiAl interface. Physical Chemistry Chemical Physics, 2016, 18, 22864-22873.	1.3	19
38	Anomalous mechanical strengths and shear deformation paths of Al₂O₃ polymorphs with high ionicity. RSC Advances, 2016, 6, 12885-12892.	1.7	8
39	Understanding the Anchoring Effect of Two-Dimensional Layered Materials for Lithiumâ€“Sulfur Batteries. Nano Letters, 2015, 15, 3780-3786.	4.5	779