Zhong-Heng Fu

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Understanding the Anchoring Effect of Two-Dimensional Layered Materials for Lithium–Sulfur Batteries. Nano Letters, 2015, 15, 3780-3786.	4.5	779
2	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. Chemical Reviews, 2019, 119, 11980-12031.	23.0	242
3	Highly Air-Stable Carbon-Based α-CsPbI ₃ Perovskite Solar Cells with a Broadened Optical Spectrum. ACS Energy Letters, 2018, 3, 1824-1831.	8.8	235
4	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
5	Theoretical Investigation of 2D Layered Materials as Protective Films for Lithium and Sodium Metal Anodes. Advanced Energy Materials, 2017, 7, 1602528.	10.2	196
6	A review on theoretical models for lithium–sulfur battery cathodes. InformaÄnÃ-Materiály, 2022, 4, .	8.5	143
7	Applying Classical, <i>Ab Initio</i> , and Machine-Learning Molecular Dynamics Simulations to the Liquid Electrolyte for Rechargeable Batteries. Chemical Reviews, 2022, 122, 10970-11021.	23.0	138
8	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
9	The carrier transition from Li atoms to Li vacancies in solid-state lithium alloy anodes. Science Advances, 2021, 7, eabi5520.	4.7	110
10	Anodeâ€Free Solidâ€ S tate Lithium Batteries: A Review. Advanced Energy Materials, 2022, 12, .	10.2	81
11	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
12	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
13	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
14	Single Atomâ€Modified Hybrid Transition Metal Carbides as Efficient Hydrogen Evolution Reaction Catalysts. Advanced Functional Materials, 2021, 31, 2104285.	7.8	42
15	The Origin of Fast Lithiumâ€ion Transport in the Inorganic Solid Electrolyte Interphase on Lithium Metal Anodes. Small Structures, 2022, 3, .	6.9	42
16	Stabilization of Ï"-phase in carbon-doped MnAl magnetic alloys. Journal of Alloys and Compounds, 2018, 755, 257-264.	2.8	36
17	Surface Electrochemical Stability and Strainâ€Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. Advanced Functional Materials, 2018, 28, 1804867.	7.8	33
18	First-principles design of strong solids: Approaches and applications. Physics Reports, 2019, 826, 1-49.	10.3	31

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19	Single-atom-Ni-decorated, nitrogen-doped carbon layers for efficient electrocatalytic CO2 reduction reaction. Electrochemistry Communications, 2020, 116, 106758.	2.3	31
20	Indirect-Direct Band Transformation of Few-Layer BiOCl under Biaxial Strain. Journal of Physical Chemistry C, 2016, 120, 8589-8594.	1.5	29
21	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
22	ADAIS: Automatic Derivation of Anisotropic Ideal Strength via high-throughput first-principles computations. Computer Physics Communications, 2019, 238, 244-253.	3.0	24
23	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. Carbon, 2018, 137, 156-164.	5.4	22
24	Stress Regulation on Atomic Bonding and Ionic Diffusivity: Mechanochemical Effects in Sulfide Solid Electrolytes. Energy & Fuels, 2021, 35, 10210-10218.	2.5	22
25	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
26	Giant heterogeneous magnetostriction induced by charge accumulation-mediated nanoinclusion formation in dual-phase nanostructured systems. Acta Materialia, 2021, 213, 116975.	3.8	20
27	Pinning effect of reactive elements on adhesion energy and adhesive strength of incoherent Al ₂ O ₃ /NiAl interface. Physical Chemistry Chemical Physics, 2016, 18, 22864-22873.	1.3	19
28	High-performance microwave absorption of hierarchical graphene-based and MWCNT-based full-carbon nanostructures. Applied Surface Science, 2019, 493, 541-550.	3.1	18
29	Two-Dimensional Carbonitride MXenes as an Efficient Electrocatalyst for Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 4477-4488.	1.5	13
30	Review on the lithium transport mechanism in solidâ€state battery materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	11
31	Domain - dependent electronic structure and optical absorption property in hybrid organic–inorganic perovskite. Physical Chemistry Chemical Physics, 2016, 18, 27358-27365.	1.3	10
32	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
33	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
34	Anomalous mechanical strengths and shear deformation paths of Al ₂ O ₃ polymorphs with high ionicity. RSC Advances, 2016, 6, 12885-12892.	1.7	8
35	Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of Ti ₂ CO ₂ and Mo ₂ CO ₂ . Physical Chemistry Chemical Physics, 2018, 20, 14608-14618.	1.3	8
36	Uniaxial magnetocrystalline anisotropy of tetragonal Mn Ga100â^' (50â€^â‰ å € ⁻ xâ€ ⁻ â‰ å € ⁻ 75) alloys. Journal of Magnetism and Magnetic Materials, 2019, 489, 165308.	1.0	8

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37	Designing ultrastrong 5d transition metal diborides with excellent stability for harsh service environments. Physical Chemistry Chemical Physics, 2019, 21, 16095-16107.	1.3	7
38	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
39	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