Zhu-Feng Hou

List of Publications by Year
in descending order

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103 papers	4,406 citations	126708 33 h-index	114278 63 g-index
104 all docs	104 docs citations	104 times ranked	6325 citing authors

#	Article	IF	Citations
1	Materials informatics-guided superior electrocatalyst: A case of pyrolysis-free single-atom coordinated with N-graphene nanomesh. Nano Energy, 2022, 94, 106868.	8.2	31
2	High-Pressure Mgâ€“Scâ€“H Phase Diagram and Its Superconductivity from First-Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 2747-2755.	1.5	17
3	The Systematic Study on the Stability and Superconductivity of Yâ€Mgâ€H Compounds under High Pressure. Advanced Theory and Simulations, 2022, 5, .	1.3	13
4	Density functional theory study of CH4 dissociation and C C coupling on W-terminated WC(0001) surface. Applied Surface Science, 2022, 591, 153128.	3.1	5
5	Charge Compensation Mechanisms and Oxygen Vacancy Formations in LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂: First-Principles Calculations. ACS Omega, 2022, 7, 14875-14886.	1.6	6
6	Metalâ€“Organic Framework-Derived Graphene Mesh: a Robust Scaffold for Highly Exposed Feâ€“N₄ Active Sites toward an Excellent Oxygen Reduction Catalyst in Acid Media. Journal of the American Chemical Society, 2022, 144, 9280-9291.	6.6	108
7	Li₈MnO₆: A Novel Cathode Material with Only Anionic Redox. ACS Applied Materials & Interfaces, 2022, 14, 29832-29843.	4.0	2
8	Realization of closed-loop optimization of epitaxial titanium nitride thin-film growth via machine learning. Materials Today Physics, 2021, 16, 100296.	2.9	22
9	Formation of oxygen vacancies in Li₂FeSiO₄: first-principles calculations. Physical Chemistry Chemical Physics, 2021, 23, 20444-20452.	1.3	3
10	Machine learning approach for the prediction of electron inelastic mean free paths. Physical Review Materials, 2021, 5, .	0.9	7
11	Weakening Intermediate Bindings on CuPd/Pd Core/shell Nanoparticles to Achieve Ptâ€Like Bifunctional Activity for Hydrogen Evolution and Oxygen Reduction Reactions. Advanced Functional Materials, 2021, 31, 2100883.	7.8	68
12	First-principles study of electronic structures and elasticity of Al2Fe3Si3. Journal of Physics Condensed Matter, 2021, 33, 195501.	0.7	10
13	Experimental Observation of Pressure-Induced Superconductivity in Layered Transition-Metal Chalcogenides (Zr,Hf)GeTe₄ Explored by a Data-Driven Approach. Chemistry of Materials, 2021, 33, 3602-3610.	3.2	8
14	Feâ€“Alâ€“Si Thermoelectric (FAST) Materials and Modules: Diffusion Couple and Machine-Learning-Assisted Materials Development. ACS Applied Materials & Interfaces, 2021, 13, 53346-53354.	4.0	10
15	Theoretical screening of VSe2 as support for enhanced electrocatalytic performance of transition-metal single atoms. Journal of Colloid and Interface Science, 2021, 590, 210-218.	5.0	28
16	Facet Engineering to Regulate Surface States of Topological Crystalline Insulator Bismuth Rhombic Dodecahedrons for Highly Energy Efficient Electrochemical CO₂ Reduction. Advanced Materials, 2021, 33, e2008373.	11.1	84
17	Effect of single-hydrogen-induced out-of-plane passivation on plasmon excitation in nanostructured graphene. Applied Surface Science, 2021, 553, 149558.	3.1	1
18	Anionic Oxygen Redox in the High-Lithium Material Li₈SnO₆. Chemistry of Materials, 2021, 33, 834-844.	3.2	10

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19	Identifying and Passivating Killer Defects in Pb-Free Double Cs₂AgBiBr₆ Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 10581-10588.	2.1	17
20	First-Principles Studies on the Formation of Oxygen Vacancies in Li₂CoSiO₄. Journal of the Electrochemical Society, 2021, 168, 110527.	1.3	2
21	High-T_c Superconducting Hydrides Formed by LaH₂₄ and YH₂₄ Cage Structures as Basic Blocks. Chemistry of Materials, 2021, 33, 9501-9507.	3.2	16
22	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in Cu₂ZnSnS₄Photoabsorbers. ACS Applied Materials & Interfaces, 2021, 13, 61365-61373.	4.0	11
23	Pyridinic nitrogen exclusively doped carbon materials as efficient oxygen reduction electrocatalysts for Zn-air batteries. Applied Catalysis B: Environmental, 2020, 261, 118234.	10.8	135
24	Rational Design of Nanoporous MoS₂/VS₂ Heteroarchitecture for Ultrahigh Performance Ammonia Sensors. Small, 2020, 16, e1901718.	5.2	67
25	Identifying the Lewis Base Chemistry in Preventing the Deposition of Metal Oxides on Ketone-Enriched Carbon Cathodes for Highly Durable Metalâ€“Air Batteries. ACS Applied Materials & Interfaces, 2020, 12, 3603-3609.	4.0	9
26	Data-driven exploration for pressure-induced superconductors using diamond anvil cell with boron-doped diamond electrodes and undoped diamond insulating layer. High Pressure Research, 2020, 40, 22-34.	0.4	8
27	Crystal Growth, Structural Analysis, and Pressure-Induced Superconductivity in a AgIn₅Se₈ Single Crystal Explored by a Data-Driven Approach. Inorganic Chemistry, 2020, 59, 325-331.	1.9	10
28	Elucidating the Influence of Sulfur Vacancies on Nonradiative Recombination Dynamics in Cu₂ZnSnS₄ Solar Absorbers. Journal of Physical Chemistry Letters, 2020, 11, 10354-10361.	2.1	13
29	Machine-learning-guided discovery of the gigantic magnetocaloric effect in HoB2 near the hydrogen liquefaction temperature. NPG Asia Materials, 2020, 12, .	3.8	84
30	Bayesian optimization based on a unified figure of merit for accelerated materials screening: A case study of halide perovskites. Science China Materials, 2020, 63, 1024-1035.	3.5	25
31	Epitaxial Growth of Rectangle Shape MoS₂ with Highly Aligned Orientation on Twofold Symmetry aâ€Plane Sapphire. Small, 2020, 16, e2000596.	5.2	53
32	Physical and chemical descriptors for predicting interfacial thermal resistance. Scientific Data, 2020, 7, 36.	2.4	9
33	Ba₆In₆Zn₄Se₁₉: a high performance infrared nonlinear optical crystal with [InSe₃]^{3â^’} trigonal planar functional motifs. Journal of Materials Chemistry C, 2020, 8, 7947-7955.	2.7	15
34	Pressure-induced superconductivity in SnSb₂Te₄. Journal of Physics Condensed Matter, 2020, 32, 235901.	0.7	5
35	Measurement of the Low-Energy Electron Inelastic Mean Free Path in Monolayer Graphene. Physical Review Applied, 2020, 13, .	1.5	10
36	Data integration for accelerated materials design via preference learning. New Journal of Physics, 2020, 22, 055001.	1.2	6

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37	Bayesian Optimization in Materials Science. Lecture Notes in Physics, 2020, , 413-426.	0.3	4
38	Ab Initio Simulation of Position-Dependent Electron Energy Loss and Its Application to the Plasmon Excitation of Nanographene. Journal of Physical Chemistry C, 2019, 123, 25341-25348.	1.5	4
39	Machine-Learning-Assisted Development and Theoretical Consideration for the Al₂Fe₃Si₃ Thermoelectric Material. ACS Applied Materials & Interfaces, 2019, 11, 11545-11554.	4.0	69
40	Porous hydrogen substituted graphyne for high capacity and ultra-stable sodium ion storage. Journal of Materials Chemistry A, 2019, 7, 11186-11194.	5.2	36
41	Unveiling the principle descriptor for predicting the electron inelastic mean free path based on a machine learning framework. Science and Technology of Advanced Materials, 2019, 20, 1090-1102.	2.8	14
42	Thermodynamic Stability Landscape of Halide Double Perovskites via Highâ€Throughput Computing and Machine Learning. Advanced Functional Materials, 2019, 29, 1807280.	7.8	131
43	Oxidizing Vacancies in Nitrogenâ€Doped Carbon Enhance Airâ€Cathode Activity. Advanced Materials, 2019, 31, e1803339.	11.1	52
44	Graphdiyne Containing Atomically Precise N Atoms for Efficient Anchoring of Lithium Ion. ACS Applied Materials & Interfaces, 2019, 11, 2608-2617.	4.0	100
45	Bayesian optimization of chemical composition: A comprehensive framework and its application to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi>Fe</mml:mi><mml:mi> -type magnet compounds. Physical Review Materials, 2019, 3, .	2.9	28
46	Structure prediction of boron-doped graphene by machine learning. Journal of Chemical Physics, 2018, 148, 241716.	1.2	46
47	Data-driven exploration of new pressure-induced superconductivity in PbBi₂Te₄. Science and Technology of Advanced Materials, 2018, 19, 909-916.	2.8	23
48	Efficient Optimization of the Performance of Mn²⁺â€Doped Kesterite Solar Cell: Machine Learning Aided Synthesis of High Efficient Cu₂(Mn,Zn)Sn(S,Se)₄ Solar Cells (Solar RRL 12â•2018). Solar Rrl, 2018, 2, 1870237.	3.1	1
49	Efficient Optimization of the Performance of Mn²⁺â€Doped Kesterite Solar Cell: Machine Learning Aided Synthesis of High Efficient Cu₂(Mn,Zn)Sn(S,Se)₄ Solar Cells. Solar Rrl, 2018, 2, 1800198.	3.1	46
50	Triazine-graphdiyne: A new nitrogen-carbonous material and its application as an advanced rechargeable battery anode. Carbon, 2018, 137, 442-450.	5.4	64
51	Influence of Encapsulated Water on Luminescence Energy, Line Width, and Lifetime of Carbon Nanotubes: Time Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 4006-4013.	2.1	21
52	Two pressure-induced superconducting transitions in SnBi₂Se₄ explored by data-driven materials search: new approach to developing novel functional materials including thermoelectric and superconducting materials. Applied Physics Express, 2018, 11, 093101.	1.1	24
53	Hierarchical Nâ€doped carbons from designed Nâ€rich polymer: Adsorbents with a recordâ€high capacity for desulfurization. AICHE Journal, 2018, 64, 3786-3793.	1.8	64
54	Breaking the scaling relations for oxygen reduction reaction on nitrogen-doped graphene by tensile strain. Carbon, 2018, 139, 129-136.	5.4	23

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55	Atomic Modulation of FeCoâ€“Nitrogenâ€“Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible Allâ€Solidâ€State Zincâ€“Air Battery. Advanced Energy Materials, 2017, 7, 1602420.	10.2	692
56	Two-Electron Oxygen Reduction on Carbon Materials Catalysts: Mechanisms and Active Sites. Journal of Physical Chemistry C, 2017, 121, 14524-14533.	1.5	89
57	Indirect Four-Electron Oxygen Reduction Reaction on Carbon Materials Catalysts in Acidic Solutions. ACS Catalysis, 2017, 7, 7908-7916.	5.5	42
58	Designing Nanostructures for Phonon Transport via Bayesian Optimization. Physical Review X, 2017, 7, .	2.8	127
59	MDTS: automatic complex materials design using Monte Carlo tree search. Science and Technology of Advanced Materials, 2017, 18, 498-503.	2.8	52
60	New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study. Scientific Reports, 2017, 7, 2011.	1.6	15
61	COMBO: An efficient Bayesian optimization library for materials science. Materials Discovery, 2016, 4, 18-21.	3.3	217
62	Mechanisms of Oxygen Reduction Reactions for Carbon Alloy Catalysts via First Principles Molecular Dynamics. Hyomen Kagaku, 2015, 36, 345-350.	0.0	0
63	Effect of Nitrogen Doping on the Migration of the Carbon Adatom and Monovacancy in Graphene. Journal of Physical Chemistry C, 2015, 119, 4922-4933.	1.5	29
64	Active Sites and Mechanisms for Oxygen Reduction Reaction on Nitrogen-Doped Carbon Alloy Catalysts: Stoneâ€“Wales Defect and Curvature Effect. Journal of the American Chemical Society, 2014, 136, 13629-13640.	6.6	273
65	Interplay between Oxidized Monovacancy and Nitrogen Doping in Graphene. Journal of Physical Chemistry C, 2014, 118, 19795-19805.	1.5	11
66	Possible Oxygen Reduction Reactions for Graphene Edges from First Principles. Journal of Physical Chemistry C, 2014, 118, 17616-17625.	1.5	56
67	NMR Chemical Shifts of ¹⁵N-Bearing Graphene. Journal of Physical Chemistry C, 2014, 118, 13929-13935.	1.5	11
68	Electronic structure of N-doped graphene with native point defects. Physical Review B, 2013, 87, .	1.1	113
69	Theoretical Characterization of X-ray Absorption, Emission, and Photoelectron Spectra of Nitrogen Doped along Graphene Edges. Journal of Physical Chemistry A, 2013, 117, 579-589.	1.1	39
70	Strength and bonding nature of superhard Z-carbon from first-principle study. AIP Advances, 2012, 2, .	0.6	7
71	Interplay between nitrogen dopants and native point defects in graphene. Physical Review B, 2012, 85, .	1.1	133
72	Effect of Hydrogen Termination on Carbon K-Edge X-ray Absorption Spectra of Nanographene. Journal of Physical Chemistry C, 2011, 115, 5392-5403.	1.5	44

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73	Elastic properties of MBH4 (M=Na, K, Rb, Cs). Physica B: Condensed Matter, 2011, 406, 2196-2199.	1.3	24
74	Selective nitrogen doping in graphene: Enhanced catalytic activity for the oxygen reduction reaction. Physical Review B, 2011, 84, .	1.1	33
75	High-Order Elastic Constants and Anharmonic Properties of NaBH ₄ : First-Principles Calculations. Chinese Physics Letters, 2011, 28, 076201.	1.3	2
76	Elastic properties and electronic structures of antiperovskite-type InNCo3 and InNNi3. Solid State Communications, 2010, 150, 1874-1879.	0.9	22
77	A Theoretical Investigation of the Structural Properties of Chemically Modified Mo-S-I Nanowires. Chinese Journal of Catalysis, 2010, 31, 739-746.	6.9	1
78	Defect States Induced by Oxygen Vacancies in Cubic SrTiO3: First-Principles Calculations. Journal of the Physical Society of Japan, 2010, 79, 114704.	0.7	57
79	Energetics and electronic structure of aluminum point defects in HfO2: A first-principles study. Journal of Applied Physics, 2009, 106, 014104.	1.1	21
80	Elastic properties and electronic structures of CdCNi3: A comparative study with MgCNi3. Solid State Sciences, 2009, 11, 251-258.	1.5	36
81	Elasticity, electronic structure, and dielectric property of cubic SrHfO₃ from firstâ€principles. Physica Status Solidi (B): Basic Research, 2009, 246, 135-139.	0.7	27
82	Moâ^'Sâ^'I Nanowires: A Promising Anode Material for Lithium-Ion Batteries. A First-Principles Study. Journal of Physical Chemistry C, 2009, 113, 18436-18440.	1.5	14
83	Elastic constants of NaBH ₄ and LiBH ₄ : Instability of Î²-LiBH ₄. Europhysics Letters, 2009, 88, 36005.	0.7	3
84	Structural stabilities, electronic structures and lithium deintercalation in LixMSiO4 (M=Mn, Fe, Co,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.4	106
85	First-principles study on the structural, elastic, and electronic properties of Î³-LiAlO2. Computational Materials Science, 2009, 46, 221-224.	1.4	26
86	Effects of Na-substitution on structural and electronic properties of Li2CoSiO4 cathode material. Transactions of Nonferrous Metals Society of China, 2009, 19, 182-186.	1.7	24
87	Atomistic modeling of the electrostatic and transport properties ofÂaÂsimplified nanoscale field effect transistor. Journal of Computational Electronics, 2008, 7, 500-508.	1.3	3
88	Firstâ€principles study of the structural stability and electronic structures of TaN. Physica Status Solidi (B): Basic Research, 2008, 245, 1580-1585.	0.7	21
89	Ab initio calculations of elastic modulus and electronic structures of cubic. Physica B: Condensed Matter, 2008, 403, 2624-2628.	1.3	38
90	Electronic structure and magnetic state of. Physica B: Condensed Matter, 2008, 403, 4232-4235.	1.3	11

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91	Effects of Cu, N, and Li intercalation on the structural stability and electronic structure of cubic Cu3N. Solid State Sciences, 2008, 10, 1651-1657.	1.5	32
92	Structural and electronic properties of cubic HfO2 surfaces. Computational Materials Science, 2008, 44, 46-52.	1.4	61
93	Al-induced reduction of the oxygen diffusion in HfO₂: anab initiostudy. Journal of Physics Condensed Matter, 2008, 20, 135206.	0.7	7
94	Effects of Y doping on the structural stability and defect properties of cubic HfO2. Journal of Applied Physics, 2008, 104, .	1.1	31
95	A rigorous surface-potential-based I-V model for undoped cylindrical nanowire MOSFETs. , 2007, , .		12
96	Effect of Al addition on the microstructure and electronic structure of HfO2 film. Journal of Applied Physics, 2007, 101, 013514.	1.1	17
97	Electronic and transport properties of graphene nanoribbons. , 2007, , .		5
98	Ab initio study on the structural and elastic properties of MAlSi (M=Ca, Sr, and Ba). Solid State Communications, 2007, 143, 425-428.	0.9	63
99	First-principles investigation of Mg(AlH4)2 complex hydride. Journal of Power Sources, 2006, 159, 111-115.	4.0	30
100	Effects of Al addition on the native defects in hafnia. Applied Physics Letters, 2006, 88, 182903.	1.5	24
101	Formation energies of lithium intercalations in AlSb, GaSb and InSb. PhysChemComm, 2003, 6, 47.	0.8	1
102	Electronic Structures of the Filled Tetrahedral Semiconductor LiMgN with a Zincblende-Type Structure. Chinese Physics Letters, 2003, 20, 114-116.	1.3	19
103	Change of Work Function of Pd, Ag, K on Al(001) as a Function of External Electric Field. Chinese Physics Letters, 2001, 18, 1111-1113.	1.3	5