

# Zhu-Feng Hou

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2427680/publications.pdf>

Version: 2024-02-01

103  
papers

4,406  
citations

126907

33  
h-index

110387

64  
g-index

104  
all docs

104  
docs citations

104  
times ranked

6325  
citing authors

#	ARTICLE	IF	CITATIONS
1	Atomic Modulation of FeCo–Nitrogen–Carbon Bifunctional Oxygen Electrodes for Rechargeable and Flexible All–Solid–State Zinc–Air Battery. <i>Advanced Energy Materials</i> , 2017, 7, 1602420.	19.5	692
2	Active Sites and Mechanisms for Oxygen Reduction Reaction on Nitrogen-Doped Carbon Alloy Catalysts: Stone–Wales Defect and Curvature Effect. <i>Journal of the American Chemical Society</i> , 2014, 136, 13629-13640.	13.7	273
3	COMBO: An efficient Bayesian optimization library for materials science. <i>Materials Discovery</i> , 2016, 4, 18-21.	3.3	217
4	Pyridinic nitrogen exclusively doped carbon materials as efficient oxygen reduction electrocatalysts for Zn-air batteries. <i>Applied Catalysis B: Environmental</i> , 2020, 261, 118234.	20.2	135
5	Interplay between nitrogen dopants and native point defects in graphene. <i>Physical Review B</i> , 2012, 85, .	3.2	133
6	Thermodynamic Stability Landscape of Halide Double Perovskites via High-Throughput Computing and Machine Learning. <i>Advanced Functional Materials</i> , 2019, 29, 1807280.	14.9	131
7	Designing Nanostructures for Phonon Transport via Bayesian Optimization. <i>Physical Review X</i> , 2017, 7, .	8.9	127
8	Electronic structure of N-doped graphene with native point defects. <i>Physical Review B</i> , 2013, 87, .	3.2	113
9	Metal–Organic Framework-Derived Graphene Mesh: a Robust Scaffold for Highly Exposed Fe–N <sub>4</sub> Active Sites toward an Excellent Oxygen Reduction Catalyst in Acid Media. <i>Journal of the American Chemical Society</i> , 2022, 144, 9280-9291.	13.7	108
10	Structural stabilities, electronic structures and lithium deintercalation in Li <sub>x</sub> MSiO <sub>4</sub> (M=Mn, Fe, Co,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	3.0	106
11	Graphdiyne Containing Atomically Precise N Atoms for Efficient Anchoring of Lithium Ion. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 2608-2617.	8.0	100
12	Two-Electron Oxygen Reduction on Carbon Materials Catalysts: Mechanisms and Active Sites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14524-14533.	3.1	89
13	Machine-learning-guided discovery of the gigantic magnetocaloric effect in HoB <sub>2</sub> near the hydrogen liquefaction temperature. <i>NPG Asia Materials</i> , 2020, 12, .	7.9	84
14	Facet Engineering to Regulate Surface States of Topological Crystalline Insulator Bismuth Rhombic Dodecahedrons for Highly Energy Efficient Electrochemical CO <sub>2</sub> Reduction. <i>Advanced Materials</i> , 2021, 33, e2008373.	21.0	84
15	Machine-Learning-Assisted Development and Theoretical Consideration for the Al <sub>2</sub> Fe <sub>3</sub> Si <sub>3</sub> Thermoelectric Material. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 11545-11554.	8.0	69
16	Weakening Intermediate Bindings on CuPd/Pd Core/shell Nanoparticles to Achieve Pt–Like Bifunctional Activity for Hydrogen Evolution and Oxygen Reduction Reactions. <i>Advanced Functional Materials</i> , 2021, 31, 2100883.	14.9	68
17	Rational Design of Nanoporous MoS <sub>2</sub> /VS <sub>2</sub> Heteroarchitecture for Ultrahigh Performance Ammonia Sensors. <i>Small</i> , 2020, 16, e1901718.	10.0	67
18	Triazine-graphdiyne: A new nitrogen-carbonous material and its application as an advanced rechargeable battery anode. <i>Carbon</i> , 2018, 137, 442-450.	10.3	64

#	ARTICLE	IF	CITATIONS
19	Hierarchical N-doped carbons from designed N-rich polymer: Adsorbents with a record-high capacity for desulfurization. <i>AIChE Journal</i> , 2018, 64, 3786-3793.	3.6	64
20	Ab initio study on the structural and elastic properties of MAISi (M=Ca, Sr, and Ba). <i>Solid State Communications</i> , 2007, 143, 425-428.	1.9	63
21	Structural and electronic properties of cubic HfO <sub>2</sub> surfaces. <i>Computational Materials Science</i> , 2008, 44, 46-52.	3.0	61
22	Defect States Induced by Oxygen Vacancies in Cubic SrTiO <sub>3</sub> : First-Principles Calculations. <i>Journal of the Physical Society of Japan</i> , 2010, 79, 114704.	1.6	57
23	Possible Oxygen Reduction Reactions for Graphene Edges from First Principles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17616-17625.	3.1	56
24	Epitaxial Growth of Rectangle Shape MoS <sub>2</sub> with Highly Aligned Orientation on Twofold Symmetry Plane Sapphire. <i>Small</i> , 2020, 16, e2000596.	10.0	53
25	MDTS: automatic complex materials design using Monte Carlo tree search. <i>Science and Technology of Advanced Materials</i> , 2017, 18, 498-503.	6.1	52
26	Oxidizing Vacancies in Nitrogen-Doped Carbon Enhance Air-Cathode Activity. <i>Advanced Materials</i> , 2019, 31, e1803339.	21.0	52
27	Structure prediction of boron-doped graphene by machine learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241716.	3.0	46
28	Efficient Optimization of the Performance of Mn <sup>2+</sup> -Doped Kesterite Solar Cell: Machine Learning Aided Synthesis of High Efficient Cu <sub>2</sub> (Mn,Zn)Sn(S,Se) <sub>4</sub> Solar Cells. <i>Solar Rrl</i> , 2018, 2, 1800198.	5.8	46
29	Effect of Hydrogen Termination on Carbon K-Edge X-ray Absorption Spectra of Nanographene. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5392-5403.	3.1	44
30	Indirect Four-Electron Oxygen Reduction Reaction on Carbon Materials Catalysts in Acidic Solutions. <i>ACS Catalysis</i> , 2017, 7, 7908-7916.	11.2	42
31	Theoretical Characterization of X-ray Absorption, Emission, and Photoelectron Spectra of Nitrogen Doped along Graphene Edges. <i>Journal of Physical Chemistry A</i> , 2013, 117, 579-589.	2.5	39
32	Ab initio calculations of elastic modulus and electronic structures of cubic. <i>Physica B: Condensed Matter</i> , 2008, 403, 2624-2628.	2.7	38
33	Elastic properties and electronic structures of CdCNi <sub>3</sub> : A comparative study with MgCNi <sub>3</sub> . <i>Solid State Sciences</i> , 2009, 11, 251-258.	3.2	36
34	Porous hydrogen substituted graphyne for high capacity and ultra-stable sodium ion storage. <i>Journal of Materials Chemistry A</i> , 2019, 7, 11186-11194.	10.3	36
35	Selective nitrogen doping in graphene: Enhanced catalytic activity for the oxygen reduction reaction. <i>Physical Review B</i> , 2011, 84, .	3.2	33
36	Effects of Cu, N, and Li intercalation on the structural stability and electronic structure of cubic Cu <sub>3</sub> N. <i>Solid State Sciences</i> , 2008, 10, 1651-1657.	3.2	32

#	ARTICLE	IF	CITATIONS
37	Effects of Y doping on the structural stability and defect properties of cubic HfO <sub>2</sub> . Journal of Applied Physics, 2008, 104, .	2.5	31
38	Materials informatics-guided superior electrocatalyst: A case of pyrolysis-free single-atom coordinated with N-graphene nanomesh. Nano Energy, 2022, 94, 106868.	16.0	31
39	First-principles investigation of Mg(AlH <sub>4</sub> ) <sub>2</sub> complex hydride. Journal of Power Sources, 2006, 159, 111-115.	7.8	30
40	Effect of Nitrogen Doping on the Migration of the Carbon Adatom and Monovacancy in Graphene. Journal of Physical Chemistry C, 2015, 119, 4922-4933.	3.1	29
41	Theoretical screening of VSe <sub>2</sub> as support for enhanced electrocatalytic performance of transition-metal single atoms. Journal of Colloid and Interface Science, 2021, 590, 210-218.	9.4	28
42	Bayesian optimization of chemical composition: A comprehensive framework and its application to $\text{Fe}_2\text{Mg}_2\text{Mn}_2\text{Si}_2$ -type magnet compounds. Physical Review Materials, 2019, 3, .	2.4	28
43	Elasticity, electronic structure, and dielectric property of cubic SrHfO <sub>3</sub> from first-principles. Physica Status Solidi (B): Basic Research, 2009, 246, 135-139.	1.5	27
44	First-principles study on the structural, elastic, and electronic properties of $\beta$ -LiAlO <sub>2</sub> . Computational Materials Science, 2009, 46, 221-224.	3.0	26
45	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.	6.3	25
46	Effects of Al addition on the native defects in hafnia. Applied Physics Letters, 2006, 88, 182903.	3.3	24
47	Effects of Na-substitution on structural and electronic properties of Li <sub>2</sub> CoSiO <sub>4</sub> cathode material. Transactions of Nonferrous Metals Society of China, 2009, 19, 182-186.	4.2	24
48	Elastic properties of MBH <sub>4</sub> (M=Na, K, Rb, Cs). Physica B: Condensed Matter, 2011, 406, 2196-2199.	2.7	24
49	Two pressure-induced superconducting transitions in SnBi <sub>2</sub> Se <sub>4</sub> explored by data-driven materials search: new approach to developing novel functional materials including thermoelectric and superconducting materials. Applied Physics Express, 2018, 11, 093101.	2.4	24
50	Data-driven exploration of new pressure-induced superconductivity in PbBi <sub>2</sub> Te <sub>4</sub> . Science and Technology of Advanced Materials, 2018, 19, 909-916.	6.1	23
51	Breaking the scaling relations for oxygen reduction reaction on nitrogen-doped graphene by tensile strain. Carbon, 2018, 139, 129-136.	10.3	23
52	Elastic properties and electronic structures of antiperovskite-type InNCo <sub>3</sub> and InNNi <sub>3</sub> . Solid State Communications, 2010, 150, 1874-1879.	1.9	22
53	Realization of closed-loop optimization of epitaxial titanium nitride thin-film growth via machine learning. Materials Today Physics, 2021, 16, 100296.	6.0	22
54	First-principles study of the structural stability and electronic structures of TaN. Physica Status Solidi (B): Basic Research, 2008, 245, 1580-1585.	1.5	21

#	ARTICLE	IF	CITATIONS
55	Energetics and electronic structure of aluminum point defects in HfO <sub>2</sub> : A first-principles study. Journal of Applied Physics, 2009, 106, 014104.	2.5	21
56	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.	4.6	21
57	Electronic Structures of the Filled Tetrahedral Semiconductor LiMgN with a Zincblende-Type Structure. Chinese Physics Letters, 2003, 20, 114-116.	3.3	19
58	Effect of Al addition on the microstructure and electronic structure of HfO <sub>2</sub> film. Journal of Applied Physics, 2007, 101, 013514.	2.5	17
59	Identifying and Passivating Killer Defects in Pb-Free Double Cs <sub>2</sub> AgBiBr <sub>6</sub> Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 10581-10588.	4.6	17
60	High-Pressure Mgâ€“Scâ€“H Phase Diagram and Its Superconductivity from First-Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 2747-2755.	3.1	17
61	High- <i>T<sub>c</sub></i> Superconducting Hydrides Formed by LaH <sub>24</sub> and YH <sub>24</sub> Cage Structures as Basic Blocks. Chemistry of Materials, 2021, 33, 9501-9507.	6.7	16
62	New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study. Scientific Reports, 2017, 7, 2011.	3.3	15
63	Ba <sub>6</sub> In <sub>6</sub> Zn <sub>4</sub> Se <sub>19</sub> : a high performance infrared nonlinear optical crystal with [InSe <sub>3</sub> ] <sup>3+</sup> trigonal planar functional motifs. Journal of Materials Chemistry C, 2020, 8, 7947-7955.	5.5	15
64	Moâˆ“Sâˆ“I Nanowires: A Promising Anode Material for Lithium-Ion Batteries. A First-Principles Study. Journal of Physical Chemistry C, 2009, 113, 18436-18440.	3.1	14
65	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.	6.1	14
66	Elucidating the Influence of Sulfur Vacancies on Nonradiative Recombination Dynamics in Cu <sub>2</sub> ZnSnS <sub>4</sub> Solar Absorbers. Journal of Physical Chemistry Letters, 2020, 11, 10354-10361.	4.6	13
67	The Systematic Study on the Stability and Superconductivity of Yâ€“Mgâ€“H Compounds under High Pressure. Advanced Theory and Simulations, 2022, 5, .	2.8	13
68	A rigorous surface-potential-based I-V model for undoped cylindrical nanowire MOSFETs. , 2007, , .		12
69	Electronic structure and magnetic state of. Physica B: Condensed Matter, 2008, 403, 4232-4235.	2.7	11
70	Interplay between Oxidized Monovacancy and Nitrogen Doping in Graphene. Journal of Physical Chemistry C, 2014, 118, 19795-19805.	3.1	11
71	NMR Chemical Shifts of <sup>15</sup> N-Bearing Graphene. Journal of Physical Chemistry C, 2014, 118, 13929-13935.	3.1	11
72	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in Cu <sub>2</sub> ZnSnS <sub>4</sub> Photoabsorbers. ACS Applied Materials & Interfaces, 2021, 13, 61365-61373.	8.0	11

#	ARTICLE	IF	CITATIONS
73	Crystal Growth, Structural Analysis, and Pressure-Induced Superconductivity in a $\text{AgIn}_{5/8}\text{Se}_{8/8}$ Single Crystal Explored by a Data-Driven Approach. <i>Inorganic Chemistry</i> , 2020, 59, 325-331.	4.0	10
74	Measurement of the Low-Energy Electron Inelastic Mean Free Path in Monolayer Graphene. <i>Physical Review Applied</i> , 2020, 13, .	3.8	10
75	First-principles study of electronic structures and elasticity of $\text{Al}_2\text{Fe}_3\text{Si}_3$ . <i>Journal of Physics Condensed Matter</i> , 2021, 33, 195501.	1.8	10
76	$\text{Fe-Al-Si}$ Thermoelectric (FAST) Materials and Modules: Diffusion Couple and Machine-Learning-Assisted Materials Development. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 53346-53354.	8.0	10
77	Anionic Oxygen Redox in the High-Lithium Material $\text{Li}_8\text{SnO}_6$ . <i>Chemistry of Materials</i> , 2021, 33, 834-844.	6.7	10
78	Identifying the Lewis Base Chemistry in Preventing the Deposition of Metal Oxides on Ketone-Enriched Carbon Cathodes for Highly Durable Metal-Air Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 3603-3609.	8.0	9
79	Physical and chemical descriptors for predicting interfacial thermal resistance. <i>Scientific Data</i> , 2020, 7, 36.	5.3	9
80	Data-driven exploration for pressure-induced superconductors using diamond anvil cell with boron-doped diamond electrodes and undoped diamond insulating layer. <i>High Pressure Research</i> , 2020, 40, 22-34.	1.2	8
81	Experimental Observation of Pressure-Induced Superconductivity in Layered Transition-Metal Chalcogenides ( $\text{Zr,HfGeTe}_4$ ) Explored by a Data-Driven Approach. <i>Chemistry of Materials</i> , 2021, 33, 3602-3610.	6.7	8
82	Al-induced reduction of the oxygen diffusion in $\text{HfO}_2$ : an <i>ab initio</i> study. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 135206.	1.8	7
83	Strength and bonding nature of superhard Z-carbon from first-principle study. <i>AIP Advances</i> , 2012, 2, .	1.3	7
84	Machine learning approach for the prediction of electron inelastic mean free paths. <i>Physical Review Materials</i> , 2021, 5, .	2.4	7
85	Data integration for accelerated materials design via preference learning. <i>New Journal of Physics</i> , 2020, 22, 055001.	2.9	6
86	Charge Compensation Mechanisms and Oxygen Vacancy Formations in $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ : First-Principles Calculations. <i>ACS Omega</i> , 2022, 7, 14875-14886.	3.5	6
87	Change of Work Function of Pd, Ag, K on Al(001) as a Function of External Electric Field. <i>Chinese Physics Letters</i> , 2001, 18, 1111-1113.	3.3	5
88	Electronic and transport properties of graphene nanoribbons. , 2007, , .		5
89	Pressure-induced superconductivity in $\text{SnSb}_2\text{Te}_4$ . <i>Journal of Physics Condensed Matter</i> , 2020, 32, 235901.	1.8	5
90	Density functional theory study of $\text{CH}_4$ dissociation and C C coupling on W-terminated WC(0001) surface. <i>Applied Surface Science</i> , 2022, 591, 153128.	6.1	5

#	ARTICLE	IF	CITATIONS
91	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.	3.1	4
92	Bayesian Optimization in Materials Science. Lecture Notes in Physics, 2020, , 413-426.	0.7	4
93	Atomistic modeling of the electrostatic and transport properties of a simplified nanoscale field effect transistor. Journal of Computational Electronics, 2008, 7, 500-508.	2.5	3
94	Elastic constants of $\text{NaBH}_4$ and $\text{LiBH}_4$ : Instability of $\text{F}^2\text{-LiBH}_4$ . Europhysics Letters, 2009, 88, 36005.	2.0	3
95	Formation of oxygen vacancies in $\text{Li}_2\text{FeSiO}_4$ : first-principles calculations. Physical Chemistry Chemical Physics, 2021, 23, 20444-20452.	2.8	3
96	High-Order Elastic Constants and Anharmonic Properties of $\text{NaBH}_4$ : First-Principles Calculations. Chinese Physics Letters, 2011, 28, 076201.	3.3	2
97	First-Principles Studies on the Formation of Oxygen Vacancies in $\text{Li}_2\text{CoSiO}_4$ . Journal of the Electrochemical Society, 2021, 168, 110527.	2.9	2
98	$\text{Li}_8\text{MnO}_6$ : A Novel Cathode Material with Only Anionic Redox. ACS Applied Materials & Interfaces, 2022, 14, 29832-29843.	8.0	2
99	Formation energies of lithium intercalations in AlSb, GaSb and InSb. PhysChemComm, 2003, 6, 47.	0.8	1
100	A Theoretical Investigation of the Structural Properties of Chemically Modified Mo-S-I Nanowires. Chinese Journal of Catalysis, 2010, 31, 739-746.	14.0	1
101	Efficient Optimization of the Performance of $\text{Mn}^{2+}$ -Doped Kesterite Solar Cell: Machine Learning Aided Synthesis of High Efficient $\text{Cu}_2(\text{Mn,Zn})\text{Sn}(\text{S,Se})_4$ Solar Cells (Solar RRL 12-2018). Solar Rrl, 2018, 2, 1870237.	5.8	1
102	Effect of single-hydrogen-induced out-of-plane passivation on plasmon excitation in nanostructured graphene. Applied Surface Science, 2021, 553, 149558.	6.1	1
103	Mechanisms of Oxygen Reduction Reactions for Carbon Alloy Catalysts via First Principles Molecular Dynamics. Hyomen Kagaku, 2015, 36, 345-350.	0.0	0