

Zhenpeng Hu

List of Publications by Year in descending order

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107
papers

7,332
citations

57631

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108
docs citations

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times ranked

11256
citing authors

#	ARTICLE	IF	CITATIONS
1	Homogeneous-like Alkyne Selective Hydrogenation Catalyzed by Cationic Nickel Confined in Zeolite. <i>CCS Chemistry</i> , 2022, 4, 949-962.	4.6	20
2	Atomic-Scale Characterization of Negative Differential Resistance in Ferroelectric Bi_2WO_6 . <i>Advanced Functional Materials</i> , 2022, 32, 2105256.	7.8	6
3	Anisotropic black phosphorene nanotube anodes afford ultrafast kinetic rate or extra capacities for Li-ion batteries. <i>Chinese Chemical Letters</i> , 2022, 33, 3842-3848.	4.8	4
4	Two-Dimensional Layered Green Phosphorus as an Anode Material for Li-Ion Batteries. <i>ACS Applied Energy Materials</i> , 2022, 5, 2184-2191.	2.5	6
5	A first-principles study on the electrochemical reaction activity of 3d transition metal single-atom catalysts in nitrogen-doped graphene: Trends and hints. <i>EScience</i> , 2022, 2, 219-226.	25.0	51
6	Pt Atom on the Wall of Atomic Layer Deposition (ALD)-Made MoS_2 Nanotubes for Efficient Hydrogen Evolution. <i>Small</i> , 2022, 18, e2105129.	5.2	29
7	Ultrathin Van der Waals Antiferromagnet CrTe_3 for Fabrication of In-Plane $\text{CrTe}_3/\text{CrTe}_2$ Monolayer Magnetic Heterostructures. <i>Advanced Materials</i> , 2022, 34, e2200236.	11.1	17
8	Complex spin Hamiltonian represented by an artificial neural network. <i>Physical Review B</i> , 2022, 105, .	1.1	8
9	V-Bridged Co_2O_3 to Eliminate Charge Transfer Barriers and Drive Lattice Oxygen Oxidation during Water-Splitting. <i>Advanced Functional Materials</i> , 2021, 31, 2008822.	7.8	40
10	Designing a Family of Aluminum-Containing Fluoroborate Crystals with Enhanced Birefringence and Second-Harmonic Generation Coefficients Based on the First-Principles Methods. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7431-7438.	1.5	3
11	Atomic Cobalt Vacancy-Cluster Enabling Optimized Electronic Structure for Efficient Water Splitting. <i>Advanced Functional Materials</i> , 2021, 31, 2101797.	7.8	26
12	Pd^{II} -Pt Tesseracts for the Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , 2021, 143, 496-503.	6.6	100
13	Activating Inert Surface Pt Single Atoms via Subsurface Doping for Oxygen Reduction Reaction. <i>Nano Letters</i> , 2021, 21, 7970-7978.	4.5	33
14	HSH-C10: A new quasi-2D carbon allotrope with a honeycomb-star-honeycomb lattice. <i>Chinese Chemical Letters</i> , 2021, .	4.8	3
15	Auxetic two-dimensional transition metal selenides and halides. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	27
16	Computational Study of a Novel 2D Ferromagnetic Metal: the Ce_2C Monolayer. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020, 14, 2000324.	1.2	2
17	Regular Arrangement of Two-Dimensional Clusters of Blue Phosphorene on $\text{Ag}(111)$. <i>Chinese Physics Letters</i> , 2020, 37, 096803.	1.3	17
18	Reaction Pathways for $\hat{1}\pm\text{-Ga}_2\text{O}_3$ and $\hat{1}^2\text{-Ga}_2\text{O}_3$ Phase Transition under Pressure up to 40 GPa: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23280-23286.	1.5	6

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19	Wellâ€Defined Singleâ€Atom Cobalt Catalyst for Electrocatalytic Flue Gas CO ₂ Reduction. Small, 2020, 16, e2001896.	5.2	85
20	Experimental Realization of Two-Dimensional Buckled Lieb Lattice. Nano Letters, 2020, 20, 2537-2543.	4.5	12
21	Reversible Potassium Intercalation in Blue Phosphoreneâ€Au Network Driven by an Electric Field. Journal of Physical Chemistry Letters, 2020, 11, 5584-5590.	2.1	5
22	Paulingâ€™s rules guided Monte Carlo search (PAMCARS): A shortcut of predicting inorganic crystal structures. Computer Physics Communications, 2020, 256, 107486.	3.0	4
23	Surface Nitrogen-Injection Engineering for High Formation Rate of CO ₂ Reduction to Formate. Nano Letters, 2020, 20, 6097-6103.	4.5	71
24	Corrugation Matters: Structure Models of Single Layer Heptazine-Based Graphitic Carbon Nitride from First-Principles Studies. Journal of Physical Chemistry C, 2020, 124, 4644-4651.	1.5	19
25	The Crucial Role of Charge Accumulation and Spin Polarization in Activating Carbonâ€Based Catalysts for Electrocatalytic Nitrogen Reduction. Angewandte Chemie, 2020, 132, 4555-4561.	1.6	8
26	The Crucial Role of Charge Accumulation and Spin Polarization in Activating Carbonâ€Based Catalysts for Electrocatalytic Nitrogen Reduction. Angewandte Chemie - International Edition, 2020, 59, 4525-4531.	7.2	149
27	Rational Design of Spinel Cobalt Vanadate Oxide Co ₂ VO ₄ for Superior Electrocatalysis. Advanced Materials, 2020, 32, e1907168.	11.1	134
28	Correlation-driven eightfold magnetic anisotropy in a two-dimensional oxide monolayer. Science Advances, 2020, 6, eaay0114.	4.7	43
29	Electronic and geometric factors affecting oxygen vacancy formation on CeO ₂ (111) surfaces: A first-principles study from trivalent metal doping cases. Applied Surface Science, 2019, 497, 143732.	3.1	14
30	Quadruple perovskite ruthenate as a highly efficient catalyst for acidic water oxidation. Nature Communications, 2019, 10, 3809.	5.8	150
31	Synthesis, structure and characterization of M(IO ₃) ₂ (HIO ₃) (M =) Tj ETQq1 1 0.784314 rgBT / Transactions, 2019, 48, 13074-13080.	1.6	7
32	Growth and theoretical study on the deep-ultraviolet transparent Î²-CsBa ₂ (PO ₃) ₅ nonlinear optical crystal. CrystEngComm, 2019, 21, 4690-4695.	1.3	8
33	using MoS_2 using G_0	1.1	15
34	General Î€Electronâ€Assisted Strategy for Ir, Pt, Ru, Pd, Fe, Ni Singleâ€Atom Electrocatalysts with Bifunctional Active Sites for Highly Efficient Water Splitting. Angewandte Chemie - International Edition, 2019, 58, 11868-11873.	7.2	229
35	General Î€Electronâ€Assisted Strategy for Ir, Pt, Ru, Pd, Fe, Ni Singleâ€Atom Electrocatalysts with Bifunctional Active Sites for Highly Efficient Water Splitting. Angewandte Chemie, 2019, 131, 11994-11999.	1.6	28
36	Single Mo ₁ (Cr ₁) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. ACS Catalysis, 2019, 9, 3419-3425.	5.5	258

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37	Chemical state of surrounding iron species affects the activity of Fe-Nx for electrocatalytic oxygen reduction. <i>Applied Catalysis B: Environmental</i> , 2019, 251, 240-246.	10.8	101
38	gt-C3N4 coordinated single atom as an efficient electrocatalyst for nitrogen reduction reaction. <i>Nano Research</i> , 2019, 12, 1181-1186.	5.8	87
39	A Dualâ€Stimuliâ€Responsive Coordination Network Featuring Reversible Wideâ€Range Luminescenceâ€Tuning Behavior. <i>Angewandte Chemie</i> , 2019, 131, 5670-5674.	1.6	24
40	The Quasiâ€Ptâ€Allotrope Catalyst: Hollow PtCo@singleâ€Atom Pt₁ on Nitrogenâ€Doped Carbon toward Superior Oxygen Reduction. <i>Advanced Functional Materials</i> , 2019, 29, 1807340.	7.8	97
41	A Dualâ€Stimuliâ€Responsive Coordination Network Featuring Reversible Wideâ€Range Luminescenceâ€Tuning Behavior. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5614-5618.	7.2	132
42	Efficient energy gap tuning for T-carbon via single atomic doping. <i>Chemical Physics</i> , 2019, 518, 69-73.	0.9	13
43	Activating Titania for Efficient Electrocatalysis by Vacancy Engineering. <i>ACS Catalysis</i> , 2018, 8, 4288-4293.	5.5	141
44	Realization of flat band with possible nontrivial topology in electronic Kagome lattice. <i>Science Advances</i> , 2018, 4, eaau4511.	4.7	131
45	Magnetic origin of phase stability in cubic $\hat{3}$ -MoN. <i>Applied Physics Letters</i> , 2018, 113, 221901.	1.5	6
46	Atomic-level structure engineering of metal oxides for high-rate oxygen intercalation pseudocapacitance. <i>Science Advances</i> , 2018, 4, eaau6261.	4.7	164
47	An amorphous tin-based nanohybrid for ultra-stable sodium storage. <i>Journal of Materials Chemistry A</i> , 2018, 6, 18920-18927.	5.2	22
48	Dirac Signature in Germanene on Semiconducting Substrate. <i>Advanced Science</i> , 2018, 5, 1800207.	5.6	59
49	Band Gap Modulated by Electronic Superlattice in Blue Phosphorene. <i>ACS Nano</i> , 2018, 12, 5059-5065.	7.3	92
50	The origin of the enhanced photocatalytic activity of carbon nitride nanotubes: a first-principles study. <i>Journal of Materials Chemistry A</i> , 2017, 5, 4827-4834.	5.2	50
51	Imaging metal-like monoclinic phase stabilized by surface coordination effect in vanadium dioxide nanobeam. <i>Nature Communications</i> , 2017, 8, 15561.	5.8	33
52	Screw dislocation-driven t-Ba₂V₂O₇ helical meso/nanosquares: microwave irradiation assisted-SDBS fabrication and their unique magnetic properties. <i>Journal of Materials Chemistry C</i> , 2017, 5, 6336-6342.	2.7	13
53	Frontispiz: Supported Rhodium Catalysts for Ammoniaâ€Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms. <i>Angewandte Chemie</i> , 2017, 129, .	1.6	0
54	Frontispiece: Supported Rhodium Catalysts for Ammoniaâ€Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms. <i>Angewandte Chemie - International Edition</i> , 2017, 56, .	7.2	0

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55	Supported Rhodium Catalysts for Ammonia-Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms. <i>Angewandte Chemie</i> , 2017, 129, 4790-4796.	1.6	27
56	Supported Rhodium Catalysts for Ammonia-Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4712-4718.	7.2	173
57	Atomically and Electronically Coupled Pt and CoO Hybrid Nanocatalysts for Enhanced Electrocatalytic Performance. <i>Advanced Materials</i> , 2017, 29, 1604607.	11.1	224
58	Synergistic Effects between Doped Nitrogen and Phosphorus in Metal-Free Cathode for Zinc-Air Battery from Covalent Organic Frameworks Coated CNT. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 44519-44528.	4.0	65
59	Activating cobalt(II) oxide nanorods for efficient electrocatalysis by strain engineering. <i>Nature Communications</i> , 2017, 8, 1509.	5.8	361
60	DFT+U Analysis on Stability of Low-Index Facets in Hexagonal LaCoO ₃ Perovskite: Effect of Co ³⁺ Spin States. <i>Chinese Journal of Chemical Physics</i> , 2017, 30, 295-302.	0.6	9
61	Water Splitting: Strongly Coupled Nafion Molecules and Ordered Porous CdS Networks for Enhanced Visible-Light Photoelectrochemical Hydrogen Evolution (Adv. Mater. 24/2016). <i>Advanced Materials</i> , 2016, 28, 4943-4943.	11.1	0
62	Hydrogen Treatment for Superparamagnetic VO ₂ Nanowires with Large Room-Temperature Magnetoresistance. <i>Angewandte Chemie</i> , 2016, 128, 8150-8154.	1.6	6
63	Hydrogen Treatment for Superparamagnetic VO ₂ Nanowires with Large Room-Temperature Magnetoresistance. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8018-8022.	7.2	37
64	Strongly Coupled Nafion Molecules and Ordered Porous CdS Networks for Enhanced Visible-Light Photoelectrochemical Hydrogen Evolution. <i>Advanced Materials</i> , 2016, 28, 4935-4942.	11.1	95
65	A first-principles study on Al-doped ZnO growth polarity on sapphire (0001) surface. <i>Europhysics Letters</i> , 2016, 114, 66003.	0.7	1
66	Engineering electrocatalytic activity in nanosized perovskite cobaltite through surface spin-state transition. <i>Nature Communications</i> , 2016, 7, 11510.	5.8	316
67	Engineering surface atomic structure of single-crystal cobalt (II) oxide nanorods for superior electrocatalysis. <i>Nature Communications</i> , 2016, 7, 12876.	5.8	568
68	Construction of a polyhedron decorated MOF with a unique network through the combination of two classic secondary building units. <i>Chemical Communications</i> , 2016, 52, 2079-2082.	2.2	36
69	Synergistic Effect of Titanate-Anatase Heterostructure and Hydrogenation-Induced Surface Disorder on Photocatalytic Water Splitting. <i>ACS Catalysis</i> , 2015, 5, 1708-1716.	5.5	92
70	In situ unravelling structural modulation across the charge-density-wave transition in vanadium disulfide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13333-13339.	1.3	24
71	A promising way to open an energy gap in bilayer graphene. <i>Nanoscale</i> , 2015, 7, 17096-17101.	2.8	13
72	Metallic mesocrystal nanosheets of vanadium nitride for high-performance all-solid-state pseudocapacitors. <i>Nano Research</i> , 2015, 8, 193-200.	5.8	50

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73	Ultrahigh Infrared Photoresponse from Core-Shell Single-Domain $\text{VO}_2/\text{VO}_2/\text{VO}_5$ Heterostructure in Nanobeam. <i>Advanced Functional Materials</i> , 2014, 24, 1821-1830.	7.8	87
74	The Key Role of van der Waals Interactions in $\text{MPC}/\text{Au}(111)$ ($\text{M} = \text{Co}, \text{Fe}, \text{H}_2$) Systems Based on First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27843-27849.	1.5	14
75	Ir Detectors: Ultrahigh Infrared Photoresponse from Core-Shell Single-Domain $\text{VO}_2/\text{VO}_2/\text{VO}_5$ Heterostructure in Nanobeam (<i>Adv. Funct. Mater.</i> 13/2014). <i>Advanced Functional Materials</i> , 2014, 24, 1820-1820.	7.8	2
76	Efficient Method for Fast Simulation of Scanning Tunneling Microscopy with a Tip Effect. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8953-8959.	1.1	7
77	Substrate engineering in stabilizing epitaxial $\text{MgO}(1\%1)$ polar ultrathin films: first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 315014.	0.7	0
78	Tunable Band Structures of Heterostructured Bilayers with Transition-Metal Dichalcogenide and MXene Monolayer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5593-5599.	1.5	147
79	Dimerization of boron dopant in diamond (100) epitaxy induced by strong pair correlation on the surface. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 045011.	0.7	3
80	The atomic structures of carbon nitride sheets for cathode oxygen reduction catalysis. <i>Journal of Chemical Physics</i> , 2013, 138, 164706.	1.2	19
81	Passivating a transition-metal surface for more uniform growth of graphene: Effect of Au alloying on $\text{Ni}(111)$. <i>Physical Review B</i> , 2013, 87, .	1.1	7
82	Coverage-dependent Orientations of $\text{Dy}@C_{82}$ Molecules on $\text{Au}(111)$ Surface. <i>Chinese Journal of Chemical Physics</i> , 2012, 25, 423-428.	0.6	5
83	Writing charge into the n -type $\text{LaAlO}_3/\text{SrTiO}_3$ interface: A theoretical study of the H_2O kinetics on the top AlO_2 surface. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	8
84	Tuning the catalytic property of nitrogen-doped graphene for cathode oxygen reduction reaction. <i>Physical Review B</i> , 2012, 85, .	1.1	81
85	Hexamethoxytribenzocoronene, a Janus Double Concave Molecule to Selectively Assemble with Fullerene C_{60} . <i>Chemistry Letters</i> , 2012, 41, 1588-1590.	0.7	4
86	Hydrodebromination and Oligomerization of Dibromomethane. <i>ACS Catalysis</i> , 2012, 2, 479-486.	5.5	28
87	Two-Dimensional Superlattice: Modulation of Band Gaps in Graphene-Based Monolayer Carbon Superlattices. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3373-3378.	2.1	60
88	Interactions in different domains of truxenone supramolecular assembly on $\text{Au}(111)$. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3980.	1.3	8
89	Halogen Adsorption on CeO_2 : The Role of Lewis Acid-Base Pairing. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6664-6671.	1.5	48
90	Chemistry of Lewis Acid-Base Pairs on Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10439-10450.	1.5	293

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91	Effect of Dopants on the Energy of Oxygen-Vacancy Formation at the Surface of Ceria: Local or Global?. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17898-17909.	1.5	118
92	Choice of U for DFT+ U Calculations for Titanium Oxides. <i>Journal of Physical Chemistry C</i> , 2011, 115, 5841-5845.	1.5	264
93	Chemistry of Doped Oxides: The Activation of Surface Oxygen and the Chemical Compensation Effect. <i>Journal of Physical Chemistry C</i> , 2011, 115, 3065-3074.	1.5	102
94	CO ₂ methanation on Ru-doped ceria. <i>Journal of Catalysis</i> , 2011, 278, 297-309.	3.1	328
95	STM characterization of size-selected V ₁ , V ₂ , VO, and VO ₂ clusters on a TiO ₂ (110)-(1 \times 1) surface at room temperature. <i>Surface Science</i> , 2011, 605, 972-976.	0.8	27
96	Scanning Tunneling Spectroscopy of Metal Phthalocyanines on a Au(111) Surface with a Ni Tip. <i>Chinese Physics Letters</i> , 2011, 28, 076802.	1.3	0
97	Methane complete and partial oxidation catalyzed by Pt-doped CeO ₂ . <i>Journal of Catalysis</i> , 2010, 273, 125-137.	3.1	186
98	Identification of metal-cage coupling in a single metallofullerene by inelastic electron tunneling spectroscopy. <i>Applied Physics Letters</i> , 2010, 96, 253110.	1.5	9
99	Electronic and Magnetic Properties of Metal Phthalocyanines on Au(111) Surface: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13650-13655.	1.5	81
100	Synthetic paramontroseite VO ₂ with good aqueous lithium-ion battery performance. <i>Chemical Communications</i> , 2008, , 3891.	2.2	102
101	Detecting a Molecule's Surface Hybrid State by an Fe-Coated Tip with a Non-s-Like Orbital. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15603-15606.	1.5	14
102	Identifying atomic geometry and electronic structure of (2 \times 3)-Sr/Si(100) surface and its initial oxidation. <i>Journal of Chemical Physics</i> , 2008, 129, 164707.	1.2	22
103	Kondo effect in single cobalt phthalocyanine molecules adsorbed on Au(111) monoatomic steps. <i>Journal of Chemical Physics</i> , 2008, 128, 234705.	1.2	44
104	Observation of Hierarchical Chiral Structures in 8-Nitrospiropyran Monolayers. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6973-6977.	1.2	23
105	Hexagonal Cu ₂ SnS ₃ with metallic character: Another category of conducting sulfides. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	85
106	Mechanism for Negative Differential Resistance in Molecular Electronic Devices: Local Orbital Symmetry Matching. <i>Physical Review Letters</i> , 2007, 99, 146803.	2.9	150
107	Quasi Chiral Phase Separation in a Two-Dimensional Orientationally Disordered System: 6-Nitrospiropyran on Au(111). <i>Journal of the American Chemical Society</i> , 2007, 129, 3857-3862.	6.6	57