

Guofeng Wang

List of Publications by Year in descending order

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103
papers

18,992
citations

22099

59
h-index

30010

103
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106
all docs

106
docs citations

106
times ranked

14955
citing authors

#	ARTICLE	IF	CITATIONS
1	Improved Oxygen Reduction Activity on Pt ₃ Ni(111) via Increased Surface Site Availability. <i>Science</i> , 2007, 315, 493-497.	6.0	3,924
2	Trends in electrocatalysis on extended and nanoscale Pt-bimetallic alloy surfaces. <i>Nature Materials</i> , 2007, 6, 241-247.	13.3	2,902
3	Atomically dispersed manganese catalysts for oxygen reduction in proton-exchange membrane fuel cells. <i>Nature Catalysis</i> , 2018, 1, 935-945.	16.1	1,075
4	Highly active atomically dispersed CoN ₄ fuel cell cathode catalysts derived from surfactant-assisted MOFs: carbon-shell confinement strategy. <i>Energy and Environmental Science</i> , 2019, 12, 250-260.	15.6	691
5	Design and Synthesis of Bimetallic Electrocatalyst with Multilayered Pt-Skin Surfaces. <i>Journal of the American Chemical Society</i> , 2011, 133, 14396-14403.	6.6	541
6	Performance enhancement and degradation mechanism identification of a single-atom Co-N-C catalyst for proton exchange membrane fuel cells. <i>Nature Catalysis</i> , 2020, 3, 1044-1054.	16.1	443
7	Metal-organic framework-derived nitrogen-doped highly disordered carbon for electrochemical ammonia synthesis using N ₂ and H ₂ O in alkaline electrolytes. <i>Nano Energy</i> , 2018, 48, 217-226.	8.2	406
8	Unveiling Active Sites of CO ₂ Reduction on Nitrogen-Coordinated and Atomically Dispersed Iron and Cobalt Catalysts. <i>ACS Catalysis</i> , 2018, 8, 3116-3122.	5.5	405
9	Highly efficient decomposition of ammonia using high-entropy alloy catalysts. <i>Nature Communications</i> , 2019, 10, 4011.	5.8	376
10	Thermally Driven Structure and Performance Evolution of Atomically Dispersed FeN ₄ Sites for Oxygen Reduction. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 18971-18980.	7.2	362
11	Reaction Pathway for Oxygen Reduction on FeN ₄ Embedded Graphene. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 452-456.	2.1	307
12	Single Cobalt Sites Dispersed in Hierarchically Porous Nanofiber Networks for Durable and High-Power PGM-Free Cathodes in Fuel Cells. <i>Advanced Materials</i> , 2020, 32, e2003577.	11.1	262
13	Atomically dispersed iron sites with a nitrogen-carbon coating as highly active and durable oxygen reduction catalysts for fuel cells. <i>Nature Energy</i> , 2022, 7, 652-663.	19.8	258
14	A density functional theory study of oxygen reduction reaction on Me-N ₄ (Me = Fe, Co, or Ni) clusters between graphitic pores. <i>Journal of Materials Chemistry A</i> , 2013, 1, 10790.	5.2	253
15	High-entropy nanoparticles: Synthesis-structure-property relationships and data-driven discovery. <i>Science</i> , 2022, 376, eabn3103.	6.0	239
16	A first principles study of oxygen reduction reaction on a Pt(111) surface modified by a subsurface transition metal M (M = Ni, Co, or Fe). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20178.	1.3	236
17	High-Entropy Metal Sulfide Nanoparticles Promise High-Performance Oxygen Evolution Reaction. <i>Advanced Energy Materials</i> , 2021, 11, 2002887.	10.2	226
18	Restoring the Nitrogen Cycle by Electrochemical Reduction of Nitrate: Progress and Prospects. <i>Small Methods</i> , 2020, 4, 2000672.	4.6	225

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19	3D porous graphitic nanocarbon for enhancing the performance and durability of Pt catalysts: a balance between graphitization and hierarchical porosity. <i>Energy and Environmental Science</i> , 2019, 12, 2830-2841.	15.6	219
20	Correlation Between Surface Chemistry and Electrocatalytic Properties of Monodisperse Pt _x Ni _{1-x} Nanoparticles. <i>Advanced Functional Materials</i> , 2011, 21, 147-152.	7.8	218
21	Comparison of Reaction Energetics for Oxygen Reduction Reactions on Pt(100), Pt(111), Pt/Ni(100), and Pt/Ni(111) Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6284-6292.	1.5	171
22	Mn- and N- doped carbon as promising catalysts for oxygen reduction reaction: Theoretical prediction and experimental validation. <i>Applied Catalysis B: Environmental</i> , 2019, 243, 195-203.	10.8	170
23	Atomically dispersed single iron sites for promoting Pt and Pt ₃ Co fuel cell catalysts: performance and durability improvements. <i>Energy and Environmental Science</i> , 2021, 14, 4948-4960.	15.6	168
24	Dual-Doping and Synergism toward High-Performance Seawater Electrolysis. <i>Advanced Materials</i> , 2021, 33, e2101425.	11.1	161
25	Surface faceting and elemental diffusion behaviour at atomic scale for alloy nanoparticles during in situ annealing. <i>Nature Communications</i> , 2015, 6, 8925.	5.8	159
26	Computationally aided, entropy-driven synthesis of highly efficient and durable multi-elemental alloy catalysts. <i>Science Advances</i> , 2020, 6, eaaz0510.	4.7	158
27	Denary oxide nanoparticles as highly stable catalysts for methane combustion. <i>Nature Catalysis</i> , 2021, 4, 62-70.	16.1	153
28	Role of Local Carbon Structure Surrounding FeN ₄ Sites in Boosting the Catalytic Activity for Oxygen Reduction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11319-11324.	1.5	150
29	Electrochemical and Computational Study of Oxygen Reduction Reaction on Nonprecious Transition Metal/Nitrogen Doped Carbon Nanofibers in Acid Medium. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1586-1596.	1.5	148
30	Atomically Dispersed Single Ni Site Catalysts for Nitrogen Reduction toward Electrochemical Ammonia Synthesis Using N ₂ and H ₂ O. <i>Small Methods</i> , 2020, 4, 1900821.	4.6	148
31	Pore-Edge Tailoring of Single-Atom Iron-Nitrogen Sites on Graphene for Enhanced CO ₂ Reduction. <i>ACS Catalysis</i> , 2020, 10, 10803-10811.	5.5	140
32	Promoting electrocatalytic CO ₂ reduction on nitrogen-doped carbon with sulfur addition. <i>Applied Catalysis B: Environmental</i> , 2019, 252, 240-249.	10.8	139
33	Atomically Dispersed Iron-Nitrogen Sites on Hierarchically Mesoporous Carbon Nanotube and Graphene Nanoribbon Networks for CO ₂ Reduction. <i>ACS Nano</i> , 2020, 14, 5506-5516.	7.3	125
34	Synthesis of Homogeneous Pt-Bimetallic Nanoparticles as Highly Efficient Electrocatalysts. <i>ACS Catalysis</i> , 2011, 1, 1355-1359.	5.5	124
35	Atomically Dispersed MnN ₄ Catalysts via Environmentally Benign Aqueous Synthesis for Oxygen Reduction: Mechanistic Understanding of Activity and Stability Improvements. <i>ACS Catalysis</i> , 2020, 10, 10523-10534.	5.5	123
36	Engineering Atomically Dispersed FeN ₄ Active Sites for CO ₂ Electroreduction. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1022-1032.	7.2	121

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37	Dynamically Unveiling Metal–Nitrogen Coordination during Thermal Activation to Design High-Efficient Atomically Dispersed CoN ₄ Active Sites. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9516-9526.	7.2	119
38	Promoting Atomically Dispersed MnN ₄ Sites <i>via</i> Sulfur Doping for Oxygen Reduction: Unveiling Intrinsic Activity and Degradation in Fuel Cells. <i>ACS Nano</i> , 2021, 15, 6886-6899.	7.3	119
39	Monte Carlo simulations of segregation in Pt-Ni catalyst nanoparticles. <i>Journal of Chemical Physics</i> , 2005, 122, 024706.	1.2	116
40	Lattice doping regulated interfacial reactions in cathode for enhanced cycling stability. <i>Nature Communications</i> , 2019, 10, 3447.	5.8	116
41	Bivalence Mn ₅ O ₈ with hydroxylated interphase for high-voltage aqueous sodium-ion storage. <i>Nature Communications</i> , 2016, 7, 13370.	5.8	109
42	Improving Pd–N–C fuel cell electrocatalysts through fluorination-driven rearrangements of local coordination environment. <i>Nature Energy</i> , 2021, 6, 1144-1153.	19.8	108
43	Boosting CO ₂ reduction on Fe-N-C with sulfur incorporation: Synergistic electronic and structural engineering. <i>Nano Energy</i> , 2020, 68, 104384.	8.2	106
44	Acid Stability and Demetalation of PGM-Free ORR Electrocatalyst Structures from Density Functional Theory: A Model for Single-Atom Catalyst–Dissolution. <i>ACS Catalysis</i> , 2020, 10, 14527-14539.	5.5	105
45	Overcoming immiscibility toward bimetallic catalyst library. <i>Science Advances</i> , 2020, 6, eaaz6844.	4.7	105
46	Dislocation nucleation facilitated by atomic segregation. <i>Nature Materials</i> , 2018, 17, 56-63.	13.3	99
47	Atomically dispersed single Ni site catalysts for high-efficiency CO ₂ electroreduction at industrial-level current densities. <i>Energy and Environmental Science</i> , 2022, 15, 2108-2119.	15.6	99
48	Efficient CO ₂ Electroreduction by Highly Dense and Active Pyridinic Nitrogen on Holey Carbon Layers with Fluorine Engineering. <i>ACS Catalysis</i> , 2019, 9, 2124-2133.	5.5	97
49	Molecular and Electronic Structures of Transition-Metal Macrocyclic Complexes as Related to Catalyzing Oxygen Reduction Reactions: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16038-16046.	1.5	92
50	Revealing Cycling Rate-Dependent Structure Evolution in Ni-Rich Layered Cathode Materials. <i>ACS Energy Letters</i> , 2018, 3, 2433-2440.	8.8	92
51	Atomic interpretation of high activity on transition metal and nitrogen-doped carbon nanofibers for catalyzing oxygen reduction. <i>Journal of Materials Chemistry A</i> , 2017, 5, 3336-3345.	5.2	88
52	Atomically Dispersed Dual-Metal Site Catalysts for Enhanced CO ₂ Reduction: Mechanistic Insight into Active Site Structures. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	83
53	Solid–Liquid Interfacial Reaction Triggered Propagation of Phase Transition from Surface into Bulk Lattice of Ni-Rich Layered Cathode. <i>Chemistry of Materials</i> , 2018, 30, 7016-7026.	3.2	80
54	In Situ Chainmail Catalyst Assembly in Low Tortuosity, Hierarchical Carbon Frameworks for Efficient and Stable Hydrogen Generation. <i>Advanced Energy Materials</i> , 2018, 8, 1801289.	10.2	79

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55	Core-Shell Nanostructured Cobalt-Platinum Electrocatalysts with Enhanced Durability. ACS Catalysis, 2018, 8, 35-42.	5.5	72
56	Atomic-level active sites of efficient imidazolate framework-derived nickel catalysts for CO ₂ reduction. Journal of Materials Chemistry A, 2019, 7, 26231-26237.	5.2	72
57	Density functional theory study of the adsorption of oxygen molecule on iron phthalocyanine and cobalt phthalocyanine. Molecular Simulation, 2008, 34, 1051-1056.	0.9	70
58	Beneficial compressive strain for oxygen reduction reaction on Pt (111) surface. Journal of Chemical Physics, 2014, 141, 124713.	1.2	66
59	Quantifying solvation energies at solid/liquid interfaces using continuum solvation methods. Molecular Simulation, 2017, 43, 420-427.	0.9	64
60	Atomic Structure Evolution of Pt-Co Binary Catalysts: Single Metal Sites versus Intermetallic Nanocrystals. Advanced Materials, 2021, 33, e2106371.	11.1	62
61	Predicting Young's modulus of nanowires from first-principles calculations on their surface and bulk materials. Journal of Applied Physics, 2008, 104, .	1.1	60
62	Thermally Driven Structure and Performance Evolution of Atomically Dispersed FeN ₄ Sites for Oxygen Reduction. Angewandte Chemie, 2019, 131, 19147-19156.	1.6	57
63	Surface Defect Dynamics in Organic-Inorganic Hybrid Perovskites: From Mechanism to Interfacial Properties. ACS Nano, 2019, 13, 12127-12136.	7.3	56
64	Unlocking the passivation nature of the cathode-air interfacial reactions in lithium ion batteries. Nature Communications, 2020, 11, 3204.	5.8	55
65	Surface oxygenation induced strong interaction between Pd catalyst and functional support for zinc-air batteries. Energy and Environmental Science, 2022, 15, 1573-1584.	15.6	49
66	Nanoindentation for measuring individual phase mechanical properties of lead free solder alloy. Journal of Materials Science: Materials in Electronics, 2008, 19, 514-521.	1.1	47
67	Correlation between oxygen adsorption energy and electronic structure of transition metal macrocyclic complexes. Journal of Chemical Physics, 2013, 139, 204306.	1.2	47
68	Mordant inspired wet-spinning of graphene fibers for high performance flexible supercapacitors. Journal of Materials Chemistry A, 2019, 7, 6869-6876.	5.2	47
69	Engineering Atomically Dispersed FeN ₄ Active Sites for CO ₂ Electroreduction. Angewandte Chemie, 2021, 133, 1035-1045.	1.6	39
70	Atomic-Scale Mechanism of Unidirectional Oxide Growth. Advanced Functional Materials, 2020, 30, 1906504.	7.8	30
71	Density functional calculation of activation energies for lattice and grain boundary diffusion in alumina. Physical Review B, 2013, 87, .	1.1	28
72	Identification of Efficient Active Sites in Nitrogen-Doped Carbon Nanotubes for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2020, 124, 8689-8696.	1.5	27

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73	Charged vacancy diffusion in chromium oxide crystal: DFT and DFT+U predictions. <i>Journal of Applied Physics</i> , 2016, 120, 215101.	1.1	25
74	Examination of Solid-Solution Phase Formation Rules for High Entropy Alloys from Atomistic Monte Carlo Simulations. <i>Jom</i> , 2015, 67, 2364-2374.	0.9	23
75	Dynamically Unveiling Metalâ€“Nitrogen Coordination during Thermal Activation to Design Highâ€“Efficient Atomically Dispersed CoN ₄ Active Sites. <i>Angewandte Chemie</i> , 2021, 133, 9602-9612.	1.6	21
76	In Situ Observation of Small-Scale Deformation in a Lead-Free Solder Alloy. <i>Journal of Electronic Materials</i> , 2009, 38, 400-409.	1.0	20
77	Potential-Dependent Mechanistic Study of Ethanol Electro-oxidation on Palladium. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 16602-16610.	4.0	20
78	Thermal Radiation Synthesis of Ultrafine Platinum Nanoclusters toward Methanol Oxidation. <i>Small Methods</i> , 2020, 4, 2000265.	4.6	16
79	Atomistic observation on diffusion-mediated friction between single-asperity contacts. <i>Nature Materials</i> , 2022, 21, 173-180.	13.3	16
80	On scaling relations of single atom catalysts for electrochemical ammonia synthesis. <i>Applied Surface Science</i> , 2021, 550, 149283.	3.1	15
81	Enhancing Catalytic Properties of Iron- and Nitrogen-Doped Carbon for Nitrogen Reduction through Structural Distortion: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 16004-16012.	1.5	14
82	Computational prediction and experimental evaluation of nitrate reduction to ammonia on rhodium. <i>Journal of Catalysis</i> , 2021, 402, 1-9.	3.1	14
83	Rapid Atomic Ordering Transformation toward Intermetallic Nanoparticles. <i>Nano Letters</i> , 2022, 22, 255-262.	4.5	12
84	Segregation induced order-disorder transition in Cu(Au) surface alloys. <i>Acta Materialia</i> , 2018, 154, 220-227.	3.8	11
85	Atomic-scale phase separation induced clustering of solute atoms. <i>Nature Communications</i> , 2020, 11, 3934.	5.8	11
86	Composition-dependent ordering transformations in Ptâ€“Fe nanoalloys. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2117899119.	3.3	10
87	Atomic-scale friction between single-asperity contacts unveiled through in situ transmission electron microscopy. <i>Nature Nanotechnology</i> , 2022, 17, 737-745.	15.6	9
88	Influence of surface segregation on magnetic properties of FePt nanoparticles. <i>Applied Physics Letters</i> , 2013, 103, 132405.	1.5	8
89	Atomic Scale Investigation of the CuPcâ€“MAPbX ₃ Interface and the Effect of Non-Stoichiometric Perovskite Films on Interfacial Structures. <i>ACS Nano</i> , 2021, 15, 14813-14821.	7.3	8
90	Atomically Dispersed Dualâ€“Metal Site Catalysts for Enhanced CO ₂ Reduction: Mechanistic Insight into Active Site Structures. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6

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91	Effect of surface steps on chemical ordering in the subsurface of Cu(Au) solid solutions. Physical Review B, 2021, 103, .	1.1	5
92	Coordination of Pre-oxidation Time and Temperature for a Better Corrosion Resistance to CO ₂ at 550Å°C. Oxidation of Metals, 2019, 91, 657-675.	1.0	4
93	Passive Oxide Film Growth Observed On the Atomic Scale. Advanced Materials Interfaces, 2022, 9, .	1.9	4
94	High precision electronic charge density determination for L1₀-ordered Î ³ -TiAl by quantitative convergent beam electron diffraction. Philosophical Magazine, 2012, 92, 4408-4424.	0.7	3
95	Coupling between bulk thermal defects and surface segregation dynamics. Physical Review B, 2021, 104, .	1.1	3
96	Atomic-Scale Mechanism of Unidirectional Oxide Growth. Advanced Functional Materials, 2019, 30, .	7.8	2
97	Modelling the Molecular Transportation of Subcutaneously Injected Salubrial. Biomedical Engineering and Computational Biology, 2011, 3, BECB.S7050.	0.8	1
98	First-principles transition state study of oxygen reduction reaction on Pt (111) surface modified by subsurface transition metals. Materials Research Society Symposia Proceedings, 2012, 1384, 1.	0.1	1
99	Observation of Solid-Liquid Interfacial Reactions Controlled Bulk Phase Transition of Ni-rich Layered Cathode. Microscopy and Microanalysis, 2018, 24, 1522-1523.	0.2	1
100	Comparison of Microstructural Evolution of Oxides Formed on F91 Martensitic Steel Upon Breakaway Oxidation at 700Å°C in Air and CO ₂ . Oxidation of Metals, 2019, 91, 463-482.	1.0	1
101	Influence of Surface Segregation on the Mechanical Property of Metallic Alloy Nanowires. Materials Research Society Symposia Proceedings, 2012, 1424, 127.	0.1	0
102	Charge Density Determination for Al-rich Composition L1o-ordered gamma-TiAl by Convergent Beam Electron Diffraction. Microscopy and Microanalysis, 2014, 20, 1492-1493.	0.2	0
103	First-Principles Calculated Structures and Carbon Binding Energies of Î ¹¹ $\left\{ \left\{ 10\text{ar}\{1\}1 \right\} \right\}$ $\text{mathord}\left\{ \left\{ \left\{ 10\text{ar}\{1\}1 \right\} \right\} \left\{ \left\{ 10\text{ar}\{1\}\text{ar}\{1\} \right\} \right\} \right\}$ Tilt Grain Boundaries in Corundum Structured Metal Oxides. Oxidation of Metals, 2020, 94, 37-49.	1.0	0