

Qiao-Hong Li

List of Publications by Year in descending order

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78
papers

3,137
citations

159585

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168389

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79
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79
docs citations

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times ranked

3931
citing authors

#	ARTICLE	IF	CITATIONS
1	Metal-Free Fluorine-Doped Carbon Electrocatalyst for CO ₂ Reduction Outcompeting Hydrogen Evolution. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9640-9644.	13.8	228
2	High-performance of nanostructured Ni/CeO ₂ catalyst on CO ₂ methanation. <i>Applied Catalysis B: Environmental</i> , 2020, 268, 118474.	20.2	226
3	Magnetic properties of nonmetal atoms absorbed MoS ₂ monolayers. <i>Applied Physics Letters</i> , 2010, 96, .	3.3	199
4	Highly chemical and thermally stable luminescent Eu ^x Tb ^{1-x} MOF materials for broad-range pH and temperature sensors. <i>Journal of Materials Chemistry C</i> , 2014, 2, 8065-8070.	5.5	163
5	Cobalt Boron Imidazolate Framework Derived Cobalt Nanoparticles Encapsulated in B/N Codoped Nanocarbon as Efficient Bifunctional Electrocatalysts for Overall Water Splitting. <i>Advanced Functional Materials</i> , 2018, 28, 1801136.	14.9	155
6	Conductive metal-organic framework nanowire arrays for electrocatalytic oxygen evolution. <i>Journal of Materials Chemistry A</i> , 2019, 7, 10431-10438.	10.3	115
7	Electrochemical preparation of metal-organic framework films for fast detection of nitro explosives. <i>Journal of Materials Chemistry A</i> , 2014, 2, 19473-19478.	10.3	111
8	Theoretical screening of efficient single-atom catalysts for nitrogen fixation based on a defective BN monolayer. <i>Nanoscale</i> , 2020, 12, 1541-1550.	5.6	95
9	A surface-mounted MOF thin film with oriented nanosheet arrays for enhancing the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 18519-18528.	10.3	92
10	Recent progress in improving the stability of copper-based catalysts for hydrogenation of carbon-oxygen bonds. <i>Catalysis Science and Technology</i> , 2018, 8, 3428-3449.	4.1	89
11	Interpenetrated Metal-Porphyrinic Framework for Enhanced Nonlinear Optical Limiting. <i>Journal of the American Chemical Society</i> , 2021, 143, 17162-17169.	13.7	85
12	Pressure-induced effects in the inorganic halide perovskite CsGeI ₃ . <i>RSC Advances</i> , 2019, 9, 3279-3284.	3.6	73
13	Atomic iridium@cobalt nanosheets for dinuclear tandem water oxidation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 8376-8383.	10.3	72
14	Metal-Free Fluorine-Doped Carbon Electrocatalyst for CO ₂ Reduction Outcompeting Hydrogen Evolution. <i>Angewandte Chemie</i> , 2018, 130, 9788-9792.	2.0	69
15	CO ₂ Overall Splitting by a Bifunctional Metal-Free Electrocatalyst. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13135-13139.	13.8	64
16	Vertically Aligned MoS ₂ with In-Plane Selectively Cleaved Mo-S Bond for Hydrogen Production. <i>Nano Letters</i> , 2021, 21, 1848-1855.	9.1	63
17	Combining a Titanium-Organic Cage and a Hydrogen-Bonded Organic Cage for Highly Effective Third-Order Nonlinear Optics. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 2920-2923.	13.8	59
18	Two cobalt(II) coordination polymers [Co ₂ (H ₂ O) ₄ (Hbidc) ₂] _n and [Co(Hbidc)] _n (Hbidc =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (1 CrystEngComm, 2009, 11, 1054.	2.6	53

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19	MOF Nanosheet Reconstructed Two-Dimensional Bionic Nanochannel for Protonic Field-Effect Transistors. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 9931-9935.	13.8	51
20	Enhancing the hydrogen evolution reaction by non-precious transition metal (Non-metal) atom doping in defective MoSi ₂ N ₄ monolayer. <i>Applied Surface Science</i> , 2021, 563, 150388.	6.1	49
21	Three-in-One: Opened Charge-transfer channel, positively shifted oxidation potential, and enhanced visible light response of g-C ₃ N ₄ photocatalyst through K and S Co-doping. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 4534-4544.	7.1	46
22	Photovoltaic Performance of Lead-Less Hybrid Perovskites from Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12638-12646.	3.1	39
23	Theoretical Study of the Reverse Water Gas Shift Reaction on Copper Modified \hat{I}^2 -Mo ₂ C(001) Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1235-1251.	3.1	39
24	Designable Al ₃₂ -Oxo Clusters with Hydroxide-like Structures: Snapshots of Boundary Hydrolysis and Optical Limiting. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 4849-4854.	13.8	39
25	Black Titanium-Oxo Clusters with Ultralow Band Gaps and Enhanced Nonlinear Optical Performance. <i>Journal of the American Chemical Society</i> , 2022, 144, 8153-8161.	13.7	39
26	Computation-predicted, stable, and inexpensive single-atom nanocatalyst Pt@Mo ₂ C – an important advanced material for H ₂ production. <i>Journal of Materials Chemistry A</i> , 2017, 5, 14658-14672.	10.3	34
27	Insights into the reaction mechanism of CO oxidative coupling to dimethyl oxalate over palladium: a combined DFT and IR study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9126-9134.	2.8	33
28	Ethylammonium as an alternative cation for efficient perovskite solar cells from first-principles calculations. <i>RSC Advances</i> , 2019, 9, 7356-7361.	3.6	33
29	Screening novel candidates for mid-IR nonlinear optical materials from I ₃ -V ₄ compounds. <i>Journal of Materials Chemistry C</i> , 2017, 5, 1963-1972.	5.5	32
30	Stable lead-free Te-based double perovskites with tunable band gaps: a first-principles study. <i>New Journal of Chemistry</i> , 2019, 43, 14892-14897.	2.8	32
31	Predicted photovoltaic performance of lead-based hybrid perovskites under the influence of a mixed-cation approach: theoretical insights. <i>Journal of Materials Chemistry C</i> , 2019, 7, 371-379.	5.5	32
32	Theoretical screening of group IIIA-VIIA elements doping to promote hydrogen evolution of MoS ₂ basal plane. <i>Applied Surface Science</i> , 2021, 542, 148535.	6.1	31
33	High-throughput screening of transition metal single-atom catalyst anchored on Janus MoSSe basal plane for hydrogen evolution reaction. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 10337-10345.	7.1	30
34	Oriented Assembly of 2D Metal-Pyridylporphyrinic Framework Films for Giant Nonlinear Optical Limiting. <i>Nano Letters</i> , 2021, 21, 10012-10018.	9.1	28
35	An effective strategy to achieve deeper coherent light for LiB ₃ O ₅ . <i>Journal of Materials Chemistry C</i> , 2016, 4, 1926-1934.	5.5	24
36	Experimental and Theoretical Studies on Effects of Structural Modification of Tin Nanoclusters for Third-Order Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2021, 60, 1885-1892.	4.0	21

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37	Direct Metal-Metal Interaction Contributions to Quadratic Hyperpolarizability: A Study on Dirhenium Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4965-4972.	2.5	20
38	N-Heterocyclic Carbene as a Surface Platform for Assembly of Homochiral Metal-Organic Framework Thin Films in Chiral Sensing. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 38357-38364.	8.0	20
39	Enhancing hydrogen evolution of MoS ₂ basal planes by combining single-boron catalyst and compressive strain. <i>Frontiers of Physics</i> , 2020, 15, 1.	5.0	20
40	Adsorption behavior of CO, CO ₂ , H ₂ , H ₂ O, NO, and O ₂ on pristine and defective 2D monolayer ferromagnetic Fe ₃ GeTe ₂ . <i>Applied Surface Science</i> , 2020, 527, 146894.	6.1	20
41	2D Boron Imidazolate Framework Nanosheets with Electrocatalytic Applications for Oxygen Evolution and Carbon Dioxide Reduction Reaction. <i>Small</i> , 2020, 16, e1907669.	10.0	20
42	Adsorption Behavior of Environmental Gas Molecules on Pristine and Defective MoSi ₂ N ₄ : Possible Application as Highly Sensitive and Reusable Gas Sensors. <i>ACS Omega</i> , 2022, 7, 8706-8716.	3.5	20
43	Solvent and Intermolecular Effects on First Hyperpolarizabilities of Organometallic Tungsten Carbonyl Complexes, A TDDFT Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7925-7932.	2.5	19
44	TM ₃ (TM = V, Fe, Mo, W) single-cluster catalyst confined on porous BN for electrocatalytic nitrogen reduction. <i>Journal of Materials Science and Technology</i> , 2022, 108, 46-53.	10.7	19
45	First-Principles Modeling of Lead-Free Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3795-3800.	3.1	18
46	Defective Fe ₃ GeTe ₂ monolayer as a promising electrocatalyst for spontaneous nitrogen reduction reaction. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6945-6954.	10.3	18
47	Synergistic Effect of Doping and Compositing on Photocatalytic Efficiency: A Case Study of La ₂ Ti ₂ O ₇ . <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 39327-39335.	8.0	17
48	Hybrid Zeolitic Imidazolate Frameworks for Promoting Electrocatalytic Oxygen Evolution via a Dual-Site Relay Mechanism. <i>Inorganic Chemistry</i> , 2021, 60, 3074-3081.	4.0	17
49	Strain-induced improvements on linear and nonlinear optical properties of SrB ₄ O ₇ crystal. <i>AIP Advances</i> , 2012, 2, 032170.	1.3	15
50	CO ₂ Overall Splitting by a Bifunctional Metal-Free Electrocatalyst. <i>Angewandte Chemie</i> , 2018, 130, 13319-13323.	2.0	15
51	Design of Hybrid Zeolitic Imidazolate Framework-Derived Material with Ca-Mo-S Triatomic Coordination for Electrochemical Oxygen Reduction. <i>Small</i> , 2021, 17, e2003256.	10.0	14
52	Atomically Precise Titanium-Oxo Nanotube with Selective Water Adsorption and Semiconductive Behaviors. <i>CCS Chemistry</i> , 2020, 2, 209-215.	7.8	14
53	Silver-Templated Keggin Alkyltin-Oxo Cluster: Electronic Structure and Optical Limiting Effect. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	14
54	A comprehensive understanding of water photooxidation on Ag ₃ PO ₄ surfaces. <i>RSC Advances</i> , 2017, 7, 23994-24003.	3.6	13

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55	Anatase TiO ₂ film composed of nanorods with predominant {110} active facets as an excellent photocatalyst for water splitting. International Journal of Hydrogen Energy, 2017, 42, 5478-5484.	7.1	13
56	Tin Metal Cluster Compounds as New Third-Order Nonlinear Optical Materials by Computational Study. Journal of Physical Chemistry Letters, 2021, 12, 7537-7544.	4.6	13
57	Novel Third-Order Nonlinear Optical Materials with Craig-Möbius Aromaticity. Journal of Physical Chemistry Letters, 2021, 12, 11784-11789.	4.6	13
58	High-Throughput computational screening of Single-atom embedded in defective BN nanotube for electrocatalytic nitrogen fixation. Applied Surface Science, 2022, 591, 153130.	6.1	13
59	Second-order nonlinear optical properties of transition metal clusters [MoS ₄ Cu ₄ X ₂ Py ₂] (M = Mo, W); Tj ETQq1 1 0,784314 ggBT /Ov	2.8	10
60	Inert Can Be Advantageous: Advisable Reconstruction and Application of Palladium Chloride for the Preferential Oxidation of the Hydrogen Impurity in Carbon Monoxide Streams. ChemCatChem, 2016, 8, 1909-1914.	3.7	10
61	Aluminium nanorings: configuration deformation and structural transformation. Chemical Communications, 2021, 57, 2085-2088.	4.1	10
62	Modulating the electronic structures and optical absorption spectra of BeO nanotubes by uniaxial strain. Applied Physics Letters, 2010, 97, 051901.	3.3	9
63	Incorporating Trialkylsilylethynyl-Substituted Head-to-Head Bithiophene Unit into Copolymers for Efficient Non-Fullerene Organic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 7271-7280.	8.0	9
64	Accelerated design of photovoltaic Ruddlesden-Popper perovskite Ca ₆ Sn ₄ S ₁₄ using machine learning. APL Materials, 2020, 8, .	5.1	9
65	Combining a Titanium Organic Cage and a Hydrogen-Bonded Organic Cage for Highly Effective Third-Order Nonlinear Optics. Angewandte Chemie, 2021, 133, 2956-2959.	2.0	9
66	Aluminum molecular rings bearing amino-polyalcohol for iodine capture. Inorganic Chemistry Frontiers, 2022, 9, 592-598.	6.0	9
67	One-step synthesis of nonstoichiometric TiO ₂ nanorod films for enhanced photocatalytic H ₂ evolution. Dalton Transactions, 2018, 47, 4478-4485.	3.3	8
68	Tunable third-order nonlinear optical effect via modifying Ti ₄ (embonate) ₆ cage-based ionic pairs. Inorganic Chemistry Frontiers, 2022, 9, 1984-1991.	6.0	8
69	Heterometallic Ag ₂ Ti ₁₀ and Ag ₄ Ti ₈ -oxo clusters with different silver doping models: synthesis, structure, and theoretical studies. Dalton Transactions, 2020, 49, 11005-11009.	3.3	7
70	The exceptionally high moisture responsiveness of a new conductive-coordination-polymer based chemiresistive sensor. CrystEngComm, 2021, 23, 3549-3556.	2.6	7
71	MOF Nanosheet Reconstructed Two-Dimensional Bionic Nanochannel for Protonic Field-Effect Transistors. Angewandte Chemie, 2021, 133, 10019-10023.	2.0	6
72	A novel Pd ₃ O ₉ @ γ -Al ₂ O ₃ catalyst under a hydroxylated effect: high activity in the CO oxidation reaction. Physical Chemistry Chemical Physics, 2015, 17, 32140-32148.	2.8	5

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73	Mechanism Insights into Second-Order Nonlinear Optical Responses of Anionic Metal Clusters. <i>Journal of Cluster Science</i> , 2011, 22, 365-380.	3.3	4
74	Functional ligand directed assembly and electronic structure of Sn ₁₈ -oxo wheel nanoclusters. <i>Chemical Communications</i> , 2021, 57, 5159-5162.	4.1	4
75	Designable Al ₃₂ -Oxo Clusters with Hydrotalcite-like Structures: Snapshots of Boundary Hydrolysis and Optical Limiting. <i>Angewandte Chemie</i> , 2021, 133, 4899-4904.	2.0	3
76	Silver-templated Keggin Alkyltin-Oxo Cluster: Electronic Structure and Optical Limiting Effect. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	1
77	Tailoring nonlinear optical crystal borophosphate through the introduction of transition metal d orbitals for improving optical anisotropy and SHG response: a first-principles investigation. <i>Materials Research Express</i> , 2018, 5, 096204.	1.6	0
78	Innen-¼-cktitelbild: Metal-Free Fluorine-Doped Carbon Electrocatalyst for CO2 Reduction Outcompeting Hydrogen Evolution (Angew. Chem. 31/2018). <i>Angewandte Chemie</i> , 2018, 130, 10133-10133.	2.0	0