List of Publications by Year in descending order

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#	Article	lF	CITATIONS
1	Real-Time, Time-Dependent Density Functional Theory Study on Photoinduced Isomerizations of Azobenzene Under a Light Field. Journal of Physical Chemistry Letters, 2022, 13, 427-432.	4.6	6
2	High-curvature carbon-supported Ni single atoms with charge polarization for highly efficient CO ₂ reduction. Chemical Communications, 2022, 58, 2914-2917.	4.1	11
3	Dual-Atom Metal and Nonmetal Site Catalyst on a Single Nickel Atom Supported on a Hybridized BCN Nanosheet for Electrochemical CO ₂ Reduction to Methane: Combining High Activity and Selectivity. ACS Applied Materials & Interfaces, 2022, 14, 9073-9083.	8.0	34
4	Toward Rational Design of Dual-Metal-Site Catalysts: Catalytic Descriptor Exploration. ACS Catalysis, 2022, 12, 3420-3429.	11.2	40
5	Zinc porphyrin and rhenium complex-based donor-acceptor conjugated porous polymer for visible-light-driven conversion of CO2 to CO. Journal of CO2 Utilization, 2022, 60, 101972.	6.8	8
6	Global Fold Switching of the RafH Protein: Diverse Structures with a Conserved Pathway. Journal of Physical Chemistry B, 2022, 126, 2979-2989.	2.6	2
7	Machine learning recognition of protein secondary structures based on two-dimensional spectroscopic descriptors. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2202713119.	7.1	16
8	Synergistic effect of a diatomic boron-doped layered two-dimensional MSi ₂ N ₄ monolayer for an efficient electrochemical nitrogen reduction. Journal of Materials Chemistry A, 2022, 10, 14820-14827.	10.3	5
9	Edge-effect enhanced catalytic CO oxidation by atomically dispersed Pt on nitride-graphene. Journal of Materials Chemistry A, 2021, 9, 2093-2098.	10.3	5
10	Spatial Confinement of a Carbon Nanocone for an Efficient Oxygen Evolution Reaction. Journal of Physical Chemistry Letters, 2021, 12, 2252-2258.	4.6	4
11	Electronic Spin Moment As a Catalytic Descriptor for Fe Single-Atom Catalysts Supported on C ₂ N. Journal of the American Chemical Society, 2021, 143, 4405-4413.	13.7	138
12	Donor–Acceptor Type Conjugated Microporous Polymer as a Metal-Free Photocatalyst for Visible-Light-Driven Aerobic Oxidative Coupling of Amines. Catalysis Letters, 2021, 151, 3145-3153.	2.6	6
13	N-Doped Graphene-Supported Diatomic Ni–Fe Catalyst for Synergistic Oxidation of CO. Journal of Physical Chemistry C, 2021, 125, 5616-5622.	3.1	23
14	Bridged Azobenzene Enables Dynamic Control of Through-Space Charge Transfer for Photochemical Conversion. Journal of Physical Chemistry Letters, 2021, 12, 3868-3874.	4.6	3
15	Modulating Charge Separation and Intersystem Crossing in Donor–Switch–Acceptor Systems: A Computational Study. Journal of Physical Chemistry A, 2021, 125, 3088-3094.	2.5	4
16	Cooperative Single-Atom Active Centers for Attenuating the Linear Scaling Effect in the Nitrogen Reduction Reaction. Journal of Physical Chemistry Letters, 2021, 12, 5233-5240.	4.6	25
17	Hydrogenated Oxide as Novel Quasi-metallic Cocatalyst for Efficient Visible-Light Driven Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2021, 125, 12672-12681.	3.1	5
18	AI-based spectroscopic monitoring of real-time interactions between SARS-CoV-2 and human ACE2. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	7

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19	Two-Dimensional All-in-One Sulfide Monolayers Driving Photocatalytic Overall Water Splitting. Nano Letters, 2021, 21, 6228-6236.	9.1	88
20	A machine learning vibrational spectroscopy protocol for spectrum prediction and spectrum-based structure recognition. Fundamental Research, 2021, 1, 488-494.	3.3	19
21	Regulating Electronic Spin Moments of Single-Atom Catalyst Sites via Single-Atom Promoter Tuning on S-Vacancy MoS ₂ for Efficient Nitrogen Fixation. Journal of Physical Chemistry Letters, 2021, 12, 8355-8362.	4.6	63
22	Facile Removal of Bulk Oxygen Vacancy Defects in Metal Oxides Driven by Hydrogen-Dopant Evaporation. Journal of Physical Chemistry Letters, 2021, 12, 9579-9583.	4.6	1
23	Accurate Machine Learning Prediction of Protein Circular Dichroism Spectra with Embedded Density Descriptors. Jacs Au, 2021, 1, 2377-2384.	7.9	16
24	A stable triplet diradical emitter. Chemical Science, 2021, 12, 15151-15156.	7.4	17
25	Imidazole-linked porphyrin-based conjugated microporous polymers for metal-free photocatalytic oxidative dehydrogenation of N-heterocycles. Sustainable Energy and Fuels, 2021, 5, 6478-6487.	4.9	6
26	Porous Metallosalen Hypercrosslinked Ionic Polymers for Cooperative CO ₂ Cycloaddition Conversion. Industrial & Engineering Chemistry Research, 2020, 59, 676-684.	3.7	34
27	Zinc porphyrin-based electron donor–acceptor-conjugated microporous polymer for the efficient photocatalytic oxidative coupling of amines under visible light. Applied Catalysis A: General, 2020, 590, 117352.	4.3	21
28	Cobalt–Salen-Based Porous Ionic Polymer: The Role of Valence on Cooperative Conversion of CO ₂ to Cyclic Carbonate. ACS Applied Materials & Interfaces, 2020, 12, 609-618.	8.0	53
29	Theoretical Calculation of Hydrogen Generation and Delivery via Photocatalytic Water Splitting in Boron–Carbon–Nitride Nanotube/Metal Cluster Hybrid. ACS Applied Materials & Interfaces, 2020, 12, 48684-48690.	8.0	6
30	Emerging linear activity trend in the oxygen evolution reaction with dual-active-sites mechanism. Journal of Materials Chemistry A, 2020, 8, 20946-20952.	10.3	17
31	Azopyrazole-Based Photoswitchable Anion Receptor for Dihydrogen Phosphate Transport. Journal of Physical Chemistry A, 2020, 124, 9692-9697.	2.5	9
32	Atomic Origin for Hydrogenation Promoted Bulk Oxygen Vacancies Removal in Vanadium Dioxide. Journal of Physical Chemistry Letters, 2020, 11, 10045-10051.	4.6	9
33	Efficient and Accurate Simulations of Vibrational and Electronic Spectra with Symmetry-Preserving Neural Network Models for Tensorial Properties. Journal of Physical Chemistry B, 2020, 124, 7284-7290.	2.6	51
34	Regulation of Electronic Structure of Graphene Nanoribbon by Tuning Long-Range Dopant–Dopant Coupling at Distance of Tens of Nanometers. Journal of Physical Chemistry Letters, 2020, 11, 6907-6913.	4.6	5
35	Realizing a Not-Strong-Not-Weak Polarization Electric Field in Single-Atom Catalysts Sandwiched by Boron Nitride and Graphene Sheets for Efficient Nitrogen Fixation. Journal of the American Chemical Society, 2020, 142, 19308-19315.	13.7	170
36	A Machine Learning Protocol for Predicting Protein Infrared Spectra. Journal of the American Chemical Society, 2020, 142, 19071-19077.	13.7	55

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37	Regulating Photocatalysis by Spin-State Manipulation of Cobalt in Covalent Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 16723-16731.	13.7	333
38	Exceeding the volcano relationship in oxygen reduction/evolution reactions using single-atom-based catalysts with dual-active-sites. Journal of Materials Chemistry A, 2020, 8, 10193-10198.	10.3	33
39	Mechanism Study of Molecular Deformation of 2,2′,5′,2″-Tetramethylated <i>p</i> -Terphenyl-4,4″-dit Trapped in Gold Junctions. Journal of Physical Chemistry Letters, 2020, 11, 4456-4461.	hiol 4.6	5
40	Synergistic Effect of Surface-Terminated Oxygen Vacancy and Single-Atom Catalysts on Defective MXenes for Efficient Nitrogen Fixation. Journal of Physical Chemistry Letters, 2020, 11, 5051-5058.	4.6	88
41	Impact of Active Site Density on Oxygen Reduction Reactions Using Monodispersed Fe–N–C Single-Atom Catalysts. ACS Applied Materials & Interfaces, 2020, 12, 15271-15278.	8.0	55
42	Biomimetic Aerobic Epoxidation of Alkenes Catalyzed by Cobalt Porphyrin under Ambient Conditions in the Presence of Sunflower Seeds Oil as a Co-Substrate. ACS Omega, 2020, 5, 4890-4899.	3.5	12
43	Sharp-tip enhanced catalytic CO oxidation by atomically dispersed Pt ₁ /Pt ₂ on a raised graphene oxide platform. Journal of Materials Chemistry A, 2020, 8, 12485-12494.	10.3	9
44	Aggregation-Induced Intersystem Crossing: Rational Design for Phosphorescence Manipulation. Journal of Physical Chemistry B, 2020, 124, 2238-2244.	2.6	29
45	Tunable Hydrogen Doping of Metal Oxide Semiconductors with Acid–Metal Treatment at Ambient Conditions. Journal of the American Chemical Society, 2020, 142, 4136-4140.	13.7	65
46	Theoretical Spectroscopic Studies on Chemical and Electronic Structures of Selenocysteine and Pyrrolysine. Journal of Physical Chemistry A, 2020, 124, 2215-2224.	2.5	3
47	Carbon Monoxide Oxidation Promoted by Surface Polarization Charges in a CuO/Ag Hybrid Catalyst. Scientific Reports, 2020, 10, 2552.	3.3	3
48	Sulfur Atomically Doped Bismuth Nanobelt Driven by Electrochemical Self-Reconstruction for Boosted Electrocatalysis. Journal of Physical Chemistry Letters, 2020, 11, 1746-1752.	4.6	23
49	Tuning Phase Transitions in Metal Oxides by Hydrogen Doping: A First-Principles Study. Journal of Physical Chemistry Letters, 2020, 11, 1075-1080.	4.6	12
50	Nickel nanograins anchored on a carbon framework for an efficient hydrogen evolution electrocatalyst and a flexible electrode. Journal of Materials Chemistry A, 2020, 8, 3499-3508.	10.3	18
51	Cooperative Nitrogen Activation and Ammonia Synthesis on Densely Monodispersed Mo–N–C Sites. Journal of Physical Chemistry Letters, 2020, 11, 3962-3968.	4.6	23
52	A Carbazolyl Porphyrinâ€Based Conjugated Microporous Polymer for Metalâ€Free Photocatalytic Aerobic Oxidation Reactions. ChemCatChem, 2020, 12, 3523-3529.	3.7	24
53	Using Machine Learning to Predict the Dissociation Energy of Organic Carbonyls. Journal of Physical Chemistry A, 2020, 124, 3844-3850.	2.5	18
54	Electric Dipole Descriptor for Machine Learning Prediction of Catalyst Surface–Molecular Adsorbate Interactions. Journal of the American Chemical Society, 2020, 142, 7737-7743.	13.7	65

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55	Enabling Efficient Charge Separation for Optoelectronic Conversion via an Energy-Dependent Z-Scheme n-Semiconductor–Metal–p-Semiconductor Schottky Heterojunction. Journal of Physical Chemistry Letters, 2020, 11, 3313-3319.	4.6	9
56	A computational study on the tunability of woven covalent organic frameworks for photocatalysis. Physical Chemistry Chemical Physics, 2019, 21, 546-553.	2.8	14
57	Role of Hydrogen Bonding in Green Fluorescent Protein-like Chromophore Emission. Scientific Reports, 2019, 9, 11640.	3.3	17
58	Energy-Dependent Z-Scheme via Metal-Interfacing Two-Dimensional p-Type and n-Type Semiconductor Layers for Efficient Optoelectronic Conversion. Journal of Physical Chemistry Letters, 2019, 10, 4317-4322.	4.6	2
59	Electron–Proton Coâ€dopingâ€Induced Metal–Insulator Transition in VO ₂ Film via Surface Selfâ€Assembled <scp>l</scp> â€Ascorbic Acid Molecules. Angewandte Chemie - International Edition, 2019, 58, 13711-13716.	13.8	27
60	Competition between dispersion interactions and conventional hydrogen bonding: insights from a theoretical study on Z-Arg-OH. Physical Chemistry Chemical Physics, 2019, 21, 17893-17900.	2.8	2
61	Electron–Proton Coâ€dopingâ€Induced Metal–Insulator Transition in VO 2 Film via Surface Selfâ€Assembled I â€Ascorbic Acid Molecules. Angewandte Chemie, 2019, 131, 13849-13854.	2.0	3
62	Enhanced Activity of C ₂ N-Supported Single Co Atom Catalyst by Single Atom Promoter. Journal of Physical Chemistry Letters, 2019, 10, 7009-7014.	4.6	35
63	Photoswitchable de/adsorption of an azobenzene-derived surfactant on a silica surface. Physical Chemistry Chemical Physics, 2019, 21, 21030-21037.	2.8	9
64	Modulating Electron Transfer in an Organic Reaction via Chemical Group Modification of the Photocatalyst. Journal of Physical Chemistry Letters, 2019, 10, 5634-5639.	4.6	5
65	Machine Learning Protocol for Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 6026-6031.	4.6	60
66	Protecting Single Atom Catalysts with Graphene/Carbon-Nitride "Chainmailâ€: Journal of Physical Chemistry Letters, 2019, 10, 3129-3133.	4.6	33
67	A neural network protocol for electronic excitations of <i>N</i> -methylacetamide. Proceedings of the United States of America, 2019, 116, 11612-11617.	7.1	55
68	Highly Selective and Efficient Synthesis of 7-Aminoquinolines and Their Applications as Golgi-Localized Probes. ACS Medicinal Chemistry Letters, 2019, 10, 954-959.	2.8	40
69	A novel energy-dependent p-semiconductor–metal–n-semiconductor heterojunction for selectively steering charge flow in a <i>Z</i> -scheme photocatalyst. Journal of Materials Chemistry A, 2019, 7, 15036-15041.	10.3	6
70	Graphene–boron nitride hybrid-supported single Mo atom electrocatalysts for efficient nitrogen reduction reaction. Journal of Materials Chemistry A, 2019, 7, 15173-15180.	10.3	107
71	Cate-controlled VO ₂ phase transition for high-performance smart windows. Science Advances, 2019, 5, eaav6815.	10.3	160
72	Promoting Intersystem Crossing of a Fluorescent Molecule via Single Functional Group Modification. Journal of Physical Chemistry Letters, 2019, 10, 1388-1393.	4.6	15

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73	Tunable Single-Photon Emission by Defective Boron-Nitride Nanotubes for High-Precision Force Detection. Journal of Physical Chemistry C, 2019, 123, 9624-9628.	3.1	5
74	Catalytic Chemistry Predicted by a Charge Polarization Descriptor: Synergistic O ₂ Activation and CO Oxidation by Au–Cu Bimetallic Clusters on TiO ₂ (101). ACS Applied Materials & Interfaces, 2019, 11, 9629-9640.	8.0	28
75	Boosted Reactivity of Ammonia Borane Dehydrogenation over Ni/Ni ₂ P Heterostructure. Journal of Physical Chemistry Letters, 2019, 10, 1048-1054.	4.6	52
76	Isolating hydrogen from oxygen in photocatalytic water splitting with a carbon-quantum-dot/carbon-nitride hybrid. Journal of Materials Chemistry A, 2019, 7, 6143-6148.	10.3	32
77	Carbon nanotube-encapsulated cobalt for oxygen reduction: integration of space confinement and N-doping. Chemical Communications, 2019, 55, 14801-14804.	4.1	85
78	Kinetic Ionic Permeation and Interfacial Doping of Supported Graphene. Nano Letters, 2019, 19, 9029-9036.	9.1	16
79	Single nickel atom supported on hybridized graphene–boron nitride nanosheet as a highly active bi-functional electrocatalyst for hydrogen and oxygen evolution reactions. Journal of Materials Chemistry A, 2019, 7, 26261-26265.	10.3	44
80	Bimetallic Pd/Co Embedded in Two-Dimensional Carbon-Nitride for Z-Scheme Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2019, 123, 1846-1851.	3.1	10
81	Bandgap tuning of C3N monolayer: A first-principles study. Chemical Physics, 2019, 520, 40-46.	1.9	19
82	Metal-Free Boron Nitride Nanoribbon Catalysts for Electrochemical CO ₂ Reduction: Combining High Activity and Selectivity. ACS Applied Materials & Interfaces, 2019, 11, 906-915.	8.0	66
83	Metal-enhanced hydrogenation of graphene with atomic pattern. Carbon, 2019, 143, 700-705.	10.3	14
84	Non-catalytic hydrogenation of VO2 in acid solution. Nature Communications, 2018, 9, 818.	12.8	87
85	Function-oriented ionic polymers having high-density active sites for sustainable carbon dioxide conversion. Journal of Materials Chemistry A, 2018, 6, 9172-9182.	10.3	91
86	Self-Adaptive Switch Enabling Complete Charge Separation in Molecular-Based Optoelectronic Conversion. Journal of Physical Chemistry Letters, 2018, 9, 837-843.	4.6	11
87	Mechanistic Understanding towards the Role of Cyclohexene in Enhancing the Efficiency of Manganese Porphyrinâ€Catalyzed Aerobic Oxidation of Diphenylmethane. European Journal of Inorganic Chemistry, 2018, 2018, 2666-2674.	2.0	16
88	CO oxidation on Ru–Pt bimetallic nanoclusters supported on TiO2(101): The effect of charge polarization. Journal of Chemical Physics, 2018, 148, 124701.	3.0	14
89	Fluorescent Molybdenum Oxide Quantum Dots and Hg ^{II} Synergistically Accelerate Cobalt Porphyrin Formation: A New Strategy for Trace Hg ^{II} Analysis. ACS Applied Nano Materials, 2018, 1, 1484-1491.	5.0	8
90	Structure-dependent luminescence of tetra-(4-pyridylphenyl)ethylene: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 41-45.	2.8	4

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91	Organic field-effect optical waveguides. Nature Communications, 2018, 9, 4790.	12.8	85
92	Graphene Oxide-Supported Transition Metal Catalysts for Di-Nitrogen Reduction. Journal of Physical Chemistry C, 2018, 122, 25441-25446.	3.1	24
93	Cooperative Spin Transition of Monodispersed FeN ₃ Sites within Graphene Induced by CO Adsorption. Journal of the American Chemical Society, 2018, 140, 15149-15152.	13.7	108
94	Aggregation-Induced Enhancement of Molecular Phosphorescence Lifetime: A First-Principle Study. Journal of Physical Chemistry C, 2018, 122, 25796-25803.	3.1	29
95	Energy Materials Design for Steering Charge Kinetics. Advanced Materials, 2018, 30, e1801988.	21.0	10
96	Photocatalytic Properties and Mechanistic Insights into Visible Lightâ€Promoted Aerobic Oxidation of Sulfides to Sulfoxides via Tin Porphyrinâ€Based Porous Aromatic Frameworks. Advanced Synthesis and Catalysis, 2018, 360, 4402-4411.	4.3	67
97	C ₂ N-supported single metal ion catalysts for HCOOH dehydrogenation. Journal of Materials Chemistry A, 2018, 6, 11105-11112.	10.3	40
98	Combining High Photocatalytic Activity and Stability via Subsurface Defects in TiO ₂ . Journal of Physical Chemistry C, 2018, 122, 17221-17227.	3.1	27
99	Material descriptors for photocatalyst/catalyst design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1369.	14.6	34
100	Charged Metalloporphyrin Polymers for Cooperative Synthesis of Cyclic Carbonates from CO ₂ under Ambient Conditions. ChemSusChem, 2017, 10, 2534-2541.	6.8	122
101	Insight into Electronic and Structural Reorganizations for Defect-Induced VO ₂ Metal–Insulator Transition. Journal of Physical Chemistry Letters, 2017, 8, 3129-3132.	4.6	24
102	Identification of the protonation site of gaseous triglycine: the cis-peptide bond conformation as the global minimum. Physical Chemistry Chemical Physics, 2017, 19, 15030-15038.	2.8	13
103	Identification of the smallest peptide with a zwitterion as the global minimum: a first-principles study on arginine-containing peptides. Physical Chemistry Chemical Physics, 2017, 19, 12117-12126.	2.8	8
104	"Healing―Effect of Graphene Oxide in Achieving Robust Dilute Ferromagnetism in Oxygen-Deficient Titanium Dioxide. Journal of Physical Chemistry C, 2017, 121, 22806-22814.	3.1	8
105	Macroscopic Wires from Fluorophore-Quencher Dyads with Long-Lived Blue Emission. Journal of Physical Chemistry A, 2017, 121, 7183-7190.	2.5	5
106	Metalloporphyrin-mediated aerobic oxidation of hydrocarbons in cumene: Co-substrate specificity and mechanistic consideration. Molecular Catalysis, 2017, 440, 36-42.	2.0	23
107	Highly Active Graphene Oxide-Supported Cobalt Single-Ion Catalyst for Chemiluminescence Reaction. Analytical Chemistry, 2017, 89, 13518-13523.	6.5	51
108	Suppressing Electron–Phonon Coupling through Laser-Induced Phase Transition. ACS Applied Materials & Interfaces, 2017, 9, 23309-23313.	8.0	18

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109	Combining photocatalytic hydrogen generation and capsule storage in graphene based sandwich structures. Nature Communications, 2017, 8, 16049.	12.8	86
110	Tuning Light Absorption in Platinum(II) Terpyridyl π-Conjugated Complexes: A First-Principle Study. Journal of Physical Chemistry A, 2017, 121, 5533-5539.	2.5	0
111	Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. Physical Chemistry Chemical Physics, 2017, 19, 32389-32397.	2.8	12
112	Graphitic carbon nitride supported single-atom catalysts for efficient oxygen evolution reaction. Chemical Communications, 2016, 52, 13233-13236.	4.1	176
113	A boron-centered radical: a potassium-crown ether stabilized boryl radical anion. Chemical Communications, 2016, 52, 12714-12716.	4.1	34
114	Direct aerobic liquid phase epoxidation of propylene catalyzed by Mn(<scp>iii</scp>) porphyrin under mild conditions: evidence for the existence of both peroxide and Mn(<scp>iv</scp>)-oxo species from in situ characterizations. RSC Advances, 2015, 5, 30014-30020.	3.6	27
115	Probing flexible conformations in molecular junctions by inelastic electron tunneling spectroscopy. AIP Advances, 2015, 5, .	1.3	4
116	New bi-functional zinc catalysts based on robust and easy-to-handle N-chelating ligands for the synthesis of cyclic carbonates from epoxides and CO ₂ under mild conditions. Green Chemistry, 2014, 16, 4179-4189.	9.0	88