Xiaoqing Lu

List of Publications by Year
in descending order

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		81900	138484
193	5,080	39	58
papers	citations	h-index	g-index

195	195	195	5540
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Metalâ€“organic framework MIL-53(Al) as a solid-phase microextraction adsorbent for the determination of 16 polycyclic aromatic hydrocarbons in water samples by gas chromatographyâ€“tandem mass spectrometry. Analyst, The, 2012, 137, 5411.	3.5	165
2	Competitive adsorption of a binary CO₂â€“CH₄ mixture in nanoporous carbons: effects of edge-functionalization. Nanoscale, 2015, 7, 1002-1012.	5.6	145
3	A â€œPreâ€Constrained Metal Twinsâ€•Strategy to Prepare Efficient Dualâ€Metalâ€Atom Catalysts for Cooperative Oxygen Electrocatalysis. Advanced Materials, 2022, 34, e2107421.	21.0	134
4	Dithiafulvenyl Unit as a New Donor for High-Efficiency Dye-Sensitized Solar Cells: Synthesis and Demonstration of a Family of Metal-Free Organic Sensitizers. Organic Letters, 2012, 14, 2214-2217.	4.6	122
5	Oneâ€step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobaltâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2021, 60, 11350-11358.	13.8	118
6	Enhancing Selective Photooxidation through Coâ€“Nx-doped Carbon Materials as Singlet Oxygen Photosensitizers. ACS Catalysis, 2017, 7, 7267-7273.	11.2	111
7	Selective selenization of mixed-linker Ni-MOFs: NiSe2@NC core-shell nano-octahedrons with tunable interfacial electronic structure for hydrogen evolution reaction. Applied Catalysis B: Environmental, 2020, 272, 118976.	20.2	111
8	Molecular simulation of CO2/CH4 adsorption in brown coal: Effect of oxygen-, nitrogen-, and sulfur-containing functional groups. Applied Surface Science, 2017, 423, 33-42.	6.1	99
9	Strategies to enhance CO₂capture and separation based on engineering absorbent materials. Journal of Materials Chemistry A, 2015, 3, 12118-12132.	10.3	98
10	Electrochemical CO₂ Reduction to C₁ Products on Single Nickel/Cobalt/Ironâ€Doped Graphitic Carbon Nitride: A DFT Study. ChemSusChem, 2019, 12, 5126-5132.	6.8	81
11	Can Polypyridyl Cu(I)-based Complexes Provide Promising Sensitizers for Dye-Sensitized Solar Cells? A Theoretical Insight into Cu(I) versus Ru(II) Sensitizers. Journal of Physical Chemistry C, 2011, 115, 3753-3761.	3.1	76
12	Design of Palladium-Doped g-C₃N₄ for Enhanced Photocatalytic Activity toward Hydrogen Evolution Reaction. ACS Applied Energy Materials, 2018, 1, 2866-2873.	5.1	76
13	Architecting a Mesoporous N-Doped Graphitic Carbon Framework Encapsulating CoTe₂ as an Efficient Oxygen Evolution Electrocatalyst. ACS Applied Materials & Interfaces, 2017, 9, 36146-36153.	8.0	73
14	Initiating an efficient electrocatalyst for water splitting via valence configuration of cobalt-iron oxide. Applied Catalysis B: Environmental, 2019, 258, 117968.	20.2	70
15	Formaldehyde oxidation on the Pt/TiO2(101) surface: A DFT investigation. Journal of Organometallic Chemistry, 2012, 704, 38-48.	1.8	68
16	Template-directed synthesis of Co2P/MoSe2 in a N-doped carbon hollow structure for efficient and stable sodium/potassium ion storage. Nano Energy, 2022, 93, 106897.	16.0	68
17	Density Functional Study of Ethanol Decomposition on Rh(111). Journal of Physical Chemistry C, 2010, 114, 21493-21503.	3.1	66
18	Fe/Fe₃C Boosts H₂O₂ Utilization for Methane Conversion Overwhelming O₂ Generation. Angewandte Chemie - International Edition, 2021, 60, 8889-8895.	13.8	66

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19	Sandwiched Cathodes Assembled from CoS₂â€Modified Carbon Clothes for Highâ€Performance Lithiumâ€Sulfur Batteries. Advanced Science, 2021, 8, e2101019.	11.2	64
20	Can N, S Cocoordination Promote Single Atom Catalyst Performance in CO₂RR? Feâ€N₂S₂ Porphyrin versus Feâ€N₄ Porphyrin. Small, 2021, 17, e2100949.	10.0	62
21	Initial Reduction of CO₂ on Pd-, Ru-, and Cu-Doped CeO₂(111) Surfaces: Effects of Surface Modification on Catalytic Activity and Selectivity. ACS Applied Materials & Interfaces, 2017, 9, 26107-26117.	8.0	61
22	The adsorption behaviour of CH4 on microporous carbons: effects of surface heterogeneity. Physical Chemistry Chemical Physics, 2014, 16, 11037.	2.8	55
23	Contemporaneous inverse manipulation of the valence configuration to preferred Co2+ and Ni3+ for enhanced overall water electrocatalysis. Applied Catalysis B: Environmental, 2021, 284, 119725.	20.2	55
24	Methanol Oxidation on Pt₃Sn(111) for Direct Methanol Fuel Cells: Methanol Decomposition. ACS Applied Materials & Interfaces, 2016, 8, 12194-12204.	8.0	52
25	Cu acting as Fe activity promoter in dual-atom Cu/Fe-NC catalyst in CO2RR to C1 products. Applied Surface Science, 2021, 564, 150423.	6.1	52
26	First-principles insight into the photoelectronic properties of Ge-based perovskites. RSC Advances, 2016, 6, 86976-86981.	3.6	51
27	DFT/TD-DFT study of novel T shaped phenothiazine-based organic dyes for dye-sensitized solar cells applications. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 212, 272-280.	3.9	51
28	Photoelectrochemical sensing of Cu2+ ions with SnO2/CdS heterostructural films. Sensors and Actuators B: Chemical, 2013, 183, 601-607.	7.8	49
29	The Oxidation of Methanol on PtRu(111): A Periodic Density Functional Theory Investigation. Journal of Physical Chemistry C, 2015, 119, 20389-20400.	3.1	49
30	Penta-graphene as a promising controllable CO2 capture and separation material in an electric field. Applied Surface Science, 2020, 502, 144067.	6.1	49
31	Single transition metal atoms on nitrogen-doped carbon for CO2 electrocatalytic reduction: CO production or further CO reduction?. Applied Surface Science, 2020, 533, 147466.	6.1	47
32	Label-free detection of 3-nitro-l-tyrosine with nickel-doped graphene localized surface plasmon resonance biosensor. Biosensors and Bioelectronics, 2017, 89, 468-476.	10.1	46
33	Coupled Heterostructure of Moâ€“Fe Selenide Nanosheets Supported on Carbon Paper as an Integrated Electrocatalyst for Efficient Hydrogen Evolution. ACS Applied Materials & Interfaces, 2018, 10, 27787-27794.	8.0	46
34	Density Functional Theory Study of the Adsorption and Desulfurization of Thiophene and Its Hydrogenated Derivatives on Pt(111): Implication for the Mechanism of Hydrodesulfurization over Noble Metal Catalysts. ACS Catalysis, 2011, 1, 1498-1510.	11.2	45
35	Nitrated tyrosine adsorption on metal-doped graphene: A DFT study. Computational Materials Science, 2012, 51, 141-145.	3.0	45
36	Achieving red/near-infrared mechanoresponsive luminescence turn-on: mechanically disturbed metastable nanostructures in organic solids. Chemical Communications, 2017, 53, 1309-1312.	4.1	45

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37	Mechanistic insights into porous graphene membranes for helium separation and hydrogen purification. Applied Surface Science, 2018, 441, 631-638.	6.1	42
38	Pdâ€“Fe3O4 Janus nanozyme with rational design for ultrasensitive colorimetric detection of biothiols. Biosensors and Bioelectronics, 2022, 196, 113724.	10.1	42
39	Methanol dehydrogenation on Rh(111): A density functional and microkinetic modeling study. Journal of Molecular Catalysis A, 2011, 344, 99-110.	4.8	41
40	DFT/TD-DFT Investigation of Electronic Structures and Spectra Properties of Cu-Based Dye Sensitizers. Journal of Physical Chemistry A, 2010, 114, 1178-1184.	2.5	40
41	Rational Design of Metallic NiTe_x (x = 1 or 2) as Bifunctional Electrocatalysts for Efficient Urea Conversion. ACS Applied Energy Materials, 2019, 2, 3363-3372.	5.1	40
42	Mechanistic insight into the hydrazine decomposition on Rh(111): effect of reaction intermediate on catalytic activity. Physical Chemistry Chemical Physics, 2013, 15, 16172.	2.8	39
43	Plasmonic enhanced dye-sensitized solar cells with self-assembly gold-TiO2@coreâ€“shell nanoislands. Solar Energy, 2014, 99, 115-125.	6.1	39
44	Stimulus-responsive adsorbent materials for CO₂ capture and separation. Journal of Materials Chemistry A, 2020, 8, 10519-10533.	10.3	39
45	An active site pre-anchoring and post-exposure strategy in Fe(CN)64-@PPy derived Fe/S/N-doped carbon electrocatalyst for high performance oxygen reduction reaction and zinc-air batteries. Chemical Engineering Journal, 2021, 413, 127395.	12.7	38
46	Facile fabrication of superhydrophobic Bi/Bi2O3 surfaces with hierarchical micro-nanostructures by electroless deposition or electrodeposition. Applied Surface Science, 2014, 288, 558-563.	6.1	36
47	Initial reduction of CO₂ on perfect and O-defective CeO₂ (111) surfaces: towards CO or COOH?. RSC Advances, 2015, 5, 97528-97535.	3.6	36
48	A facile co-precipitation synthesis of robust FeCo phosphate electrocatalysts for efficient oxygen evolution. Electrochimica Acta, 2018, 264, 244-250.	5.2	36
49	Computational Investigation on the Effect of Graphene Oxide Sheets as Nanofillers in Poly(vinyl) Tj ETQq1 1 0.784314 rgBT /Overlock	3.1	35
50	Does the Co+-assisted decarbonylation of acetaldehyde occur via Câ€“C or Câ€“H activation? A theoretical investigation using density functional theory. Chemical Physics Letters, 2005, 414, 28-33.	2.6	34
51	Tetra-carbazole substituted spiro[fluorene-9,9â€²-xanthene]-based hole-transporting materials with high thermal stability and mobility for efficient OLEDs. Dyes and Pigments, 2017, 139, 764-771.	3.7	33
52	Two Birds with One Stone: Contemporaneously Boosting OER Activity and Kinetics for Layered Double Hydroxide Inspired by Photosystem II. Advanced Functional Materials, 2022, 32, .	14.9	33
53	Mechanism of the Ethylene Conversion to Ethylidyne on Rh(111): A Density Functional Investigation. Journal of Physical Chemistry C, 2010, 114, 8440-8448.	3.1	31
54	Dehydrogenation of methanol on Pd(100): comparison with the results of Pd(111). Physical Chemistry Chemical Physics, 2010, 12, 7794.	2.8	30

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55	Theoretical Investigation of the Fe⁺-Catalyzed Oxidation of Acetylene by N₂O. Journal of Physical Chemistry A, 2008, 112, 5676-5683.	2.5	29
56	Strain-controlled carbon nitride: A continuously tunable membrane for gas separation. Applied Surface Science, 2020, 506, 144675.	6.1	29
57	Carbon Quantum Dots Promote Coupled Valence Engineering of V₂O₅ Nanobelts for Highâ€Performance Aqueous Zincâ€Ion Batteries. ChemSusChem, 2021, 14, 2076-2083.	6.8	29
58	Synthesis and Properties of Dithiafulvenyl Functionalized Spiro[fluorene-9,9â€²-xanthene] Molecules. Organic Letters, 2018, 20, 780-783.	4.6	28
59	Highly Specific Colorimetric Probe for Fluoride by Triggering the Intrinsic Catalytic Activity of a Agptâ€“Fe₃O₄ Hybrid Nanozyme Encapsulated in SiO₂ Shells. Environmental Science & Technology, 2022, 56, 1713-1723.	10.0	28
60	Theoretical Investigation of the Decarbonylation of Acetaldehyde by Fe+ and Cr+. ChemPhysChem, 2006, 7, 1345-1354.	2.1	27
61	Facile fabrication of porous thin films of Bi2O3/Bi2S3 nanocomposite semiconductors at gas/liquid interface and their photoelectrochemical performances. Applied Surface Science, 2014, 299, 131-135.	6.1	27
62	Direct tuning of meso-/micro-porous structure of carbon nanofibers confining Sb nanocrystals for advanced sodium and potassium storage. Journal of Alloys and Compounds, 2020, 833, 155127.	5.5	27
63	Promotion of electrochemical CO2 reduction to ethylene on phosphorus-doped copper nanocrystals with stable Cuδ+ sites. Applied Surface Science, 2021, 544, 148965.	6.1	27
64	Theoretical investigation on electrocatalytic reduction of CO2 to methanol and methane by bimetallic atoms TM1/TM2-N@Gra (TMÂ=ÂFe, Co, Ni, Cu). Applied Surface Science, 2022, 593, 153377.	6.1	27
65	Theoretical investigation of Câ€“H activation in Mg+â€“CH3X (X=H, NH2 and CHO). Computational and Theoretical Chemistry, 2006, 764, 177-186.	1.5	26
66	A planar dithiafulvene based sensitizer forming J -aggregates on TiO 2 photoanode to enhance the performance of dye-sensitized solar cells. Dyes and Pigments, 2017, 136, 97-103.	3.7	26
67	Fe/Fe₃C Boosts H₂O₂ Utilization for Methane Conversion Overwhelming O₂ Generation. Angewandte Chemie, 2021, 133, 8971-8977.	2.0	26
68	Novel heteroatom sulfur porphyrin organic polymer as a metal-free electrocatalyst for acidic oxygen reduction reaction. Electrochimica Acta, 2021, 377, 138107.	5.2	26
69	Composition-Tuned Surface Binding on CuZn-Ni Catalysts Boosts CO₂RR Selectivity toward CO Generation. , 2022, 4, 497-504.		26
70	Ethanoldecomposition on a Pd(110) surface: a density functional theory investigation. Dalton Transactions, 2013, 42, 2309-2318.	3.3	25
71	Effect of the functionalized Ï€-bridge on porphyrin sensitizers for dye-sensitized solar cells: an in-depth analysis of electronic structure, spectrum, excitation, and intramolecular electron transfer. Journal of Materials Chemistry C, 2015, 3, 10129-10139.	5.5	25
72	Edge-functionalized nanoporous carbons for high adsorption capacity and selectivity of CO2 over N2. Applied Surface Science, 2017, 410, 259-266.	6.1	25

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73	Nanoporous Boron Nitride Membranes for Helium Separation. ACS Applied Nano Materials, 2019, 2, 4471-4479.	5.0	25
74	Oxygen-Doped VS₄ Microspheres with Abundant Sulfur Vacancies as a Superior Electrocatalyst for the Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2020, 8, 15055-15064.	6.7	25
75	Initial Hydrogenations of Pyridine on MoP(001): A Density Functional Study. Langmuir, 2012, 28, 3129-3137.	3.5	24
76	Alkyl amine functionalized triphenylamine-based covalent organic frameworks for high-efficiency CO2 capture and separation over N2. Materials Letters, 2018, 230, 28-31.	2.6	24
77	How can the Dualâ€atom Catalyst FeCoâ€“NC Surpass Singleâ€atom Catalysts Feâ€“NC/Coâ€“NC in CO₂RR? â€“ CO Intermediate Assisted Promotion via a Synergistic Effect. Energy and Environmental Materials, 2023, 6, .	12.8	24
78	1, 3-Indanedione functionalized fluorene luminophores: Negative solvatochromism, nanostructure-morphology determined AIE and mechanoresponsive luminescence turn-on. Dyes and Pigments, 2018, 155, 225-232.	3.7	23
79	Theoretical Survey of the Thiophene Hydrodesulfurization Mechanism on Clean and Single-Sulfur-Atom-Modified MoP(001). Journal of Physical Chemistry C, 2016, 120, 23009-23023.	3.1	22
80	Rational design of TiO2@ nitrogen-doped carbon coaxial nanotubes as anode for advanced lithium ion batteries. Applied Surface Science, 2018, 458, 1018-1025.	6.1	22
81	Theoretical study of T shaped phenothiazine/carbazole based organic dyes with naphthalimide as Ï€-spacer for DSSCs. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 233, 118201.	3.9	22
82	Boosting oxygen evolution reaction of hierarchical spongy NiFe-PBA/Ni3C(B) electrocatalyst: Interfacial engineering with matchable structure. Chemical Engineering Journal, 2022, 433, 133524.	12.7	22
83	Carbon phosphides: promising electric field controllable nanoporous materials for CO₂ capture and separation. Journal of Materials Chemistry A, 2020, 8, 9970-9980.	10.3	21
84	Oneâ€step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobaltâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie, 2021, 133, 11451-11459.	2.0	21
85	First-row transition metal embedded pyrazine-based graphynes as high-performance single atom catalysts for the CO₂reduction reaction. Journal of Materials Chemistry A, 2022, 10, 9048-9058.	10.3	21
86	Decomposition of Methanthiol on Pt(111): A Density Functional Investigation. Langmuir, 2010, 26, 12017-12025.	3.5	20
87	Decomposition mechanism of methylamine to hydrogen cyanide on Pt(111): selectivity of the Câ€“H, Nâ€“H and Câ€“N bond scissions. RSC Advances, 2014, 4, 12266.	3.6	19
88	Linear thiophene-containing Ï€-conjugated aldehydes with aggregation-induced emission for building solid red luminophors. Dyes and Pigments, 2015, 115, 166-171.	3.7	19
89	Theoretical insight into electronic structure and optoelectronic properties of heteroleptic Cu(I)-based complexes for dye-sensitized solar cells. Materials Chemistry and Physics, 2016, 173, 139-145.	4.0	19
90	Theoretical investigation on the hydrogen evolution reaction mechanism at MoS₂ heterostructures: the essential role of the 1T/2H phase interface. Catalysis Science and Technology, 2020, 10, 458-465.	4.1	19

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91	Theoretical design of push-pull porphyrin dyes with Ï€-bridge modification for dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 332, 232-240.	3.9	18
92	In Situ Coupling Reconstruction of Cobaltâ€“Iron Oxide on a Cobalt Phosphate Nanoarray with Interfacial Electronic Features for Highly Enhanced Water Oxidation Catalysis. ACS Sustainable Chemistry and Engineering, 2020, 8, 4773-4780.	6.7	18
93	Theoretical analysis of the conversion mechanism of acetylene to ethylidyne on Pt(111). Physical Chemistry Chemical Physics, 2012, 14, 5642.	2.8	17
94	Mechanistic Insight into Catalytic Oxidation of Ammonia on Clean, Oâ€•and OHâ€Assisted Ir(1â€‰1â€‰1) Surfaces. ChemCatChem, 2013, 5, 1832-1841.	3.7	17
95	CO tolerance of a Pt₃Sn(111) catalyst in ethanol decomposition. Catalysis Science and Technology, 2015, 5, 3246-3258.	4.1	17
96	Competitive adsorption of CO2/CH4 in porous boron nitride nanomaterials. Materials Letters, 2015, 161, 545-548.	2.6	17
97	Diffusion and separation of CH4/N2 in pillared graphene nanomaterials: A molecular dynamics investigation. Chemical Physics Letters, 2016, 660, 272-276.	2.6	17
98	Effect of alloying on the stabilities and catalytic properties of Agâ€“Au bimetallic subnanoclusters: a theoretical investigation. Journal of Materials Science, 2016, 51, 5046-5060.	3.7	17
99	Heteroleptic Cu(I) complexes integrating functionalized chromophores for dye-sensitized solar cells: An in-depth analysis of electronic structure, spectrum, excitation, and intramolecular electron transfer. Organic Electronics, 2016, 29, 142-150.	2.6	17
100	Li-modified nanoporous carbons for high-performance adsorption and separation of CO2 over N2: A combined DFT and GCMC computational study. Journal of CO2 Utilization, 2018, 26, 588-594.	6.8	17
101	Micelles of Mesoporous Silica with Inserted Iron Complexes as a Platform for Constructing Efficient Electrocatalysts for Oxygen Reduction. ACS Applied Materials & Interfaces, 2020, 12, 54720-54731.	8.0	17
102	First-row transition-metal-doped graphyne for ultrahigh-performance CO2 capture and separation over N2/CH4/H2. Materials Today Physics, 2021, 16, 100301.	6.0	17
103	The oxidation pathways of Ti+ by acetaldehyde in the gas phase: A density functional theory investigation. Chemical Physics Letters, 2006, 431, 56-61.	2.6	16
104	Methanol oxidation on Ru(0001) for direct methanol fuel cells: analysis of the competitive reaction mechanism. RSC Advances, 2016, 6, 1729-1737.	3.6	16
105	CO2 capture and separation over N2 and CH4 in nanoporous MFM-300(In, Al, Ga, and In-3N): Insight from GCMC simulations. Journal of CO2 Utilization, 2018, 28, 145-151.	6.8	16
106	Theoretical Analysis on Heteroleptic Cu(I)-Based Complexes for Dye-Sensitized Solar Cells: Effect of Anchors on Electronic Structure, Spectrum, Excitation, and Intramolecular and Interfacial Electron Transfer. Molecules, 2020, 25, 3681.	3.8	16
107	Surface self-reconstruction of telluride induced by in-situ cathodic electrochemical activation for enhanced water oxidation performance. Applied Catalysis B: Environmental, 2022, 310, 121355.	20.2	16
108	Gas-Phase Reactions of Co+ with Ethylamine: A Theoretical Approach to the Reaction Mechanisms of Transition Metal Ions with Primary Amines. Journal of Physical Chemistry A, 2008, 112, 5312-5321.	2.5	15

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109	Theoretical insight into the desulfurization of thiophene on Pt(110): A density functional investigation. Journal of Molecular Catalysis A, 2012, 363-364, 18-25.	4.8	15
110	Regulation of dithiafulvene-based molecular shape and aggregation on TiO₂ for high efficiency dye-sensitized solar cells. Journal of Materials Chemistry C, 2019, 7, 1974-1981.	5.5	15
111	Constructing surface vacancy to activate the stuck MXenes for high-performance CO2 reduction reaction. Journal of CO2 Utilization, 2022, 62, 102074.	6.8	15
112	Facile control of surface reconstruction with Co2+ or Co3+-rich (oxy)hydroxide surface on ZnCo phosphate for large-current-density hydrogen evolution in alkali. Materials Today Physics, 2021, 20, 100448.	6.0	14
113	Efficient platinum harvesting of MOF-derived N-doped carbon through cathodic cyclic voltammetry for hydrogen evolution. Electrochimica Acta, 2019, 317, 173-181.	5.2	13
114	Metastable marcasite NiSe₂ nanodendrites on carbon fiber clothes to suppress polysulfide shuttling for high-performance lithiumâ€“sulfur batteries. Nanoscale, 2021, 13, 16487-16498.	5.6	13
115	Effects of core moiety and substituted positions in phenothiazine-based hole transporting materials towards high thermal stability and good hole mobility. Tetrahedron, 2017, 73, 7115-7121.	1.9	12
116	Enhancing the intermolecular singlet fission efficiency by controlling the self-assembly of amphipathic tetracene derivatives in aqueous solution. Journal of Materials Chemistry C, 2019, 7, 11090-11098.	5.5	12
117	Facile synthesis of an antimony-doped Cu/Cu₂O catalyst with robust CO production in a broad range of potentials for CO₂ electrochemical reduction. Journal of Materials Chemistry A, 2021, 9, 23234-23242.	10.3	12
118	Interfacial Moâ€“Nâ€“C Bond Endowed Hydrogen Evolution Reaction on MoSe₂@N-Doped Carbon Hollow Nanoflowers. Inorganic Chemistry, 2021, 60, 12377-12385.	4.0	12
119	Conversion of Amorphous MOF Microspheres into a Nickel Phosphate Battery-Type Electrode Using the â€œAnticollapseâ€•Two-Step Strategy. Inorganic Chemistry, 2021, 60, 17094-17102.	4.0	12
120	Analysis of Petroleum Aromatics by Laser-Induced Acoustic Desorption/Tunable Synchrotron Vacuum Ultraviolet Photoionization Mass Spectrometry. Energy & Fuels, 2013, 27, 2010-2017.	5.1	11
121	Hydrodenitrogenation of pyridine on MoP(010): Competition between hydrogenation and denitrification. Inorganica Chimica Acta, 2015, 435, 30-37.	2.4	11
122	Impact of diverse active sites on MoS2 catalyst: Competition on active site formation and selectivity of thiophene hydrodesulfurization reaction. Molecular Catalysis, 2019, 463, 67-76.	2.0	11
123	High-efficiency CO2 capture and separation over N2 in penta-graphene pores: insights from GCMC and DFT simulations. Journal of Materials Science, 2020, 55, 16603-16611.	3.7	11
124	Tunable rare-earth metalâ^'organic frameworks for ultra-high selenite capture. Journal of Hazardous Materials, 2022, 436, 129094.	12.4	11
125	Triple-atom catalysts 3TM-GYs (TMÂ=ÂCu, Fe, and Co; GYÂ=Âgraphyne) for high-performance CO2 reduction reaction to C1 products. Applied Materials Today, 2021, 25, 101245.	4.3	10
126	Theoretical characterization of ruthenium complexes containing functionalized bithiophene ligands for dye-sensitized solar cells. Journal of Organometallic Chemistry, 2011, 696, 1632-1639.	1.8	9

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127	On the Gas-Phase Co+-Mediated Oxidation of Ethane by N2O: A Mechanistic Study. Journal of Physical Chemistry A, 2012, 116, 3282-3289.	2.5	9
128	The Competitive Oâ€“H versus Câ€“H Bond Activation of Ethanol and Methanol by VO₂⁺ in Gas Phase: A DFT Study. Journal of Physical Chemistry A, 2013, 117, 5161-5170.	2.5	9
129	Blacking of nano-CdS thin film from gas/liquid interface for enhanced photoelectrochemical performances. Applied Surface Science, 2014, 313, 26-30.	6.1	9
130	Unraveling the Mechanism of the Zn-Improved Catalytic Activity of Pd-Based Catalysts for Waterâ€“Gas Shift Reaction. Journal of Physical Chemistry C, 2016, 120, 20181-20191.	3.1	9
131	Dithiafulvene-based organic sensitizers using pyridine as the acceptor for dye-sensitized solar cells. Materials Chemistry and Physics, 2017, 192, 349-355.	4.0	9
132	Ultrahigh Hydrogen Uptake in an Interpenetrated Zn ₄ O-Based Metalâ€“Organic Framework. CCS Chemistry, 2022, 4, 832-837.	7.8	9
133	Rational Design and Effective Control of Goldâ€Based Bimetallic Electrocatalyst for Boosting CO₂ Reduction Reaction: A Firstâ€Principles Study. ChemSusChem, 2021, 14, 2731-2739.	6.8	9
134	Tuning singlet fission in amphipathic tetracene nanoparticles by controlling the molecular packing with side-group engineering. Materials Chemistry Frontiers, 2020, 4, 2113-2125.	5.9	9
135	Cu(I)-Based Sensitizers Featuring 6,6â€²-Dimethyl-4,4â€²-Dicarboxylate-2,2â€²-Bipyridine with Functionalized 2,9-Dimethyl-1,10-Phenanthroline Ligands: A Structural, Electronic and Spectral Investigation. Science of Advanced Materials, 2015, 7, 1361-1367.	0.7	9
136	Single-Atom-like B-N₃ Sites in Ordered Macroporous Carbon for Efficient Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2021, 13, 53892-53903.	8.0	9
137	Hydrothermal synthesis of ammonium vanadate [(NH4)2V7O16â€¢3.6H2O] as a promising zinc-ion cathode: Experimental and theoretical study of its storage. Electrochimica Acta, 2022, 404, 139785.	5.2	9
138	Experimental and Computational Studies of Intracomplex Reactions in Mg+(Primary, Secondary) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3 6392-6406.	3.3	8
139	Hydride abstraction of methylamine with Cu+(1S) in the gas phase: A density functional theory study. Journal of Organometallic Chemistry, 2007, 692, 3796-3803.	1.8	8
140	Theoretical study of the gas-phase Fe+-mediated oxidation of ethane by N2O. Theoretical Chemistry Accounts, 2011, 128, 349-358.	1.4	8
141	The properties of the bonding between CO and ZIF-8 structures: a density functional theory study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	8
142	The decisive effect of interface states on the photocatalytic activity of the silver(I) oxide/titanium dioxide heterojunction. Journal of Colloid and Interface Science, 2017, 492, 167-175.	9.4	8
143	Trivacancy and Stone-Wales defected silicene for adsorption of small gas molecules. Computational Materials Science, 2018, 154, 276-283.	3.0	8
144	Theoretical Investigation on Copper(I) Complexes Featuring a Phosphonic Acid Anchor with Asymmetric Ligands for DSSC. ACS Applied Electronic Materials, 2020, 2, 2141-2150.	4.3	8

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