

Xiaoqing Lu

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184
papers

3,093
citations

31
h-index

45
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195
ext. papers

4,051
ext. citations

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avg. IF

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L-index

#	Paper	IF	Citations
184	Metal-organic framework MIL-53(Al) as a solid-phase microextraction adsorbent for the determination of 16 polycyclic aromatic hydrocarbons in water samples by gas chromatography-tandem mass spectrometry. <i>Analyst, The</i> , 2012 , 137, 5411-9	5	146
183	Dithiafulvenyl unit as a new donor for high-efficiency dye-sensitized solar cells: synthesis and demonstration of a family of metal-free organic sensitizers. <i>Organic Letters</i> , 2012 , 14, 2214-7	6.2	116
182	Competitive adsorption of a binary CO ₂ -CH ₄ mixture in nanoporous carbons: effects of edge-functionalization. <i>Nanoscale</i> , 2015 , 7, 1002-12	7.7	114
181	Strategies to enhance CO ₂ capture and separation based on engineering absorbent materials. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 12118-12132	13	87
180	Can Polypyridyl Cu(I)-based Complexes Provide Promising Sensitizers for Dye-Sensitized Solar Cells? A Theoretical Insight into Cu(I) versus Ru(II) Sensitizers. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 3753-3761	3.8	62
179	Selective selenization of mixed-linker Ni-MOFs: NiSe ₂ @NC core-shell nano-octahedrons with tunable interfacial electronic structure for hydrogen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2020 , 272, 118976	21.8	60
178	Molecular simulation of CO ₂ /CH ₄ adsorption in brown coal: Effect of oxygen-, nitrogen-, and sulfur-containing functional groups. <i>Applied Surface Science</i> , 2017 , 423, 33-42	6.7	56
177	Enhancing Selective Photooxidation through Co ^{III} -doped Carbon Materials as Singlet Oxygen Photosensitizers. <i>ACS Catalysis</i> , 2017 , 7, 7267-7273	13.1	55
176	Density Functional Study of Ethanol Decomposition on Rh(111). <i>Journal of Physical Chemistry C</i> , 2010 , 114, 21493-21503	3.8	55
175	Formaldehyde oxidation on the Pt/TiO ₂ (101) surface: A DFT investigation. <i>Journal of Organometallic Chemistry</i> , 2012 , 704, 38-48	2.3	51
174	Initial Reduction of CO on Pd-, Ru-, and Cu-Doped CeO(111) Surfaces: Effects of Surface Modification on Catalytic Activity and Selectivity. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 26107-26117	9.5	49
173	Design of Palladium-Doped g-C ₃ N ₄ for Enhanced Photocatalytic Activity toward Hydrogen Evolution Reaction. <i>ACS Applied Energy Materials</i> , 2018 , 1, 2866-2873	6.1	48
172	Initiating an efficient electrocatalyst for water splitting via valence configuration of cobalt-iron oxide. <i>Applied Catalysis B: Environmental</i> , 2019 , 258, 117968	21.8	47
171	Methanol Oxidation on Pt ₃ Sn(111) for Direct Methanol Fuel Cells: Methanol Decomposition. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 12194-204	9.5	47
170	Architecting a Mesoporous N-Doped Graphitic Carbon Framework Encapsulating CoTe as an Efficient Oxygen Evolution Electrocatalyst. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 36146-36153	9.5	44
169	The adsorption behaviour of CH ₄ on microporous carbons: effects of surface heterogeneity. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 11037-46	3.6	43
168	Nitrated tyrosine adsorption on metal-doped graphene: A DFT study. <i>Computational Materials Science</i> , 2012 , 51, 141-145	3.2	40

167	Photoelectrochemical sensing of Cu ²⁺ ions with SnO ₂ /CdS heterostructural films. <i>Sensors and Actuators B: Chemical</i> , 2013 , 183, 601-607	8.5	39
166	Mechanistic insight into the hydrazine decomposition on Rh(111): effect of reaction intermediate on catalytic activity. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 16172-82	3.6	39
165	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. <i>ACS Catalysis</i> , 2011 , 1, 1498-1510	13.1	37
164	First-principles insight into the photoelectronic properties of Ge-based perovskites. <i>RSC Advances</i> , 2016 , 6, 86976-86981	3.7	36
163	Label-free detection of 3-nitro-L-tyrosine with nickel-doped graphene localized surface plasmon resonance biosensor. <i>Biosensors and Bioelectronics</i> , 2017 , 89, 468-476	11.8	35
162	The Oxidation of Methanol on PtRu(111): A Periodic Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 20389-20400	3.8	35
161	Electrochemical CO Reduction to C Products on Single Nickel/Cobalt/Iron-Doped Graphitic Carbon Nitride: A DFT Study. <i>ChemSusChem</i> , 2019 , 12, 5126-5132	8.3	35
160	Plasmonic enhanced dye-sensitized solar cells with self-assembly gold-TiO ₂ @core-shell nanoislands. <i>Solar Energy</i> , 2014 , 99, 115-125	6.8	35
159	Methanol dehydrogenation on Rh(111): A density functional and microkinetic modeling study. <i>Journal of Molecular Catalysis A</i> , 2011 , 344, 99-110		35
158	Achieving red/near-infrared mechanoresponsive luminescence turn-on: mechanically disturbed metastable nanostructures in organic solids. <i>Chemical Communications</i> , 2017 , 53, 1309-1312	5.8	34
157	DFT/TD-DFT investigation of electronic structures and spectra properties of Cu-based dye sensitizers. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 1178-84	2.8	34
156	Does the Co ⁺ -assisted decarbonylation of acetaldehyde occur via C=O or C-H activation? A theoretical investigation using density functional theory. <i>Chemical Physics Letters</i> , 2005 , 414, 28-33	2.5	34
155	Penta-graphene as a promising controllable CO ₂ capture and separation material in an electric field. <i>Applied Surface Science</i> , 2020 , 502, 144067	6.7	32
154	Mechanistic insights into porous graphene membranes for helium separation and hydrogen purification. <i>Applied Surface Science</i> , 2018 , 441, 631-638	6.7	31
153	Facile fabrication of superhydrophobic Bi/Bi ₂ O ₃ surfaces with hierarchical micro-nanostructures by electroless deposition or electrodeposition. <i>Applied Surface Science</i> , 2014 , 288, 558-563	6.7	31
152	Coupled Heterostructure of Mo-Fe Selenide Nanosheets Supported on Carbon Paper as an Integrated Electrocatalyst for Efficient Hydrogen Evolution. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 27787-27794	9.5	30
151	Tetra-carbazole substituted spiro[fluorene-9,9'-xanthene]-based hole-transporting materials with high thermal stability and mobility for efficient OLEDs. <i>Dyes and Pigments</i> , 2017 , 139, 764-771	4.6	29
150	Mechanism of the Ethylene Conversion to Ethylidyne on Rh(111): A Density Functional Investigation. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8440-8448	3.8	29

149	Computational Investigation on the Effect of Graphene Oxide Sheets as Nanofillers in Poly(vinyl alcohol)/Graphene Oxide Composites. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 22532-22538	3.8	28
148	Theoretical investigation of the Fe ⁺ -catalyzed oxidation of acetylene by N ₂ O. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 5676-83	2.8	28
147	Dehydrogenation of methanol on Pd(100): comparison with the results of Pd(111). <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7794-803	3.6	27
146	Rational Design of Metallic NiTex (x = 1 or 2) as Bifunctional Electrocatalysts for Efficient Urea Conversion. <i>ACS Applied Energy Materials</i> , 2019 , 2, 3363-3372	6.1	26
145	A facile co-precipitation synthesis of robust FeCo phosphate electrocatalysts for efficient oxygen evolution. <i>Electrochimica Acta</i> , 2018 , 264, 244-250	6.7	26
144	Theoretical investigation of the decarbonylation of acetaldehyde by Fe ⁺ and Cr ⁺ . <i>ChemPhysChem</i> , 2006 , 7, 1345-54	3.2	26
143	Synthesis and Properties of Dithiafulvenyl Functionalized Spiro[fluorene-9,9Naphthalene] Molecules. <i>Organic Letters</i> , 2018 , 20, 780-783	6.2	24
142	Theoretical investigation of C≡N activation in Mg+TiH ₃ X (X=H, NH ₂ and CHO). <i>Computational and Theoretical Chemistry</i> , 2006 , 764, 177-186		24
141	One-step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobalt-Functionalized Metal-Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 11350-11358	16.4	24
140	Edge-functionalized nanoporous carbons for high adsorption capacity and selectivity of CO ₂ over N ₂ . <i>Applied Surface Science</i> , 2017 , 410, 259-266	6.7	23
139	Effect of the functionalized bridge on porphyrin sensitizers for dye-sensitized solar cells: an in-depth analysis of electronic structure, spectrum, excitation, and intramolecular electron transfer. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 10129-10139	7.1	23
138	Facile fabrication of porous thin films of Bi ₂ O ₃ /Bi ₂ S ₃ nanocomposite semiconductors at gas/liquid interface and their photoelectrochemical performances. <i>Applied Surface Science</i> , 2014 , 299, 131-135	6.7	23
137	Contemporaneous inverse manipulation of the valence configuration to preferred Co ²⁺ and Ni ³⁺ for enhanced overall water electrocatalysis. <i>Applied Catalysis B: Environmental</i> , 2021 , 284, 119725	21.8	23
136	DFT/TD-DFT study of novel T shaped phenothiazine-based organic dyes for dye-sensitized solar cells applications. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 212, 272-280	4.6	22
135	A planar dithiafulvene based sensitizer forming J-aggregates on TiO ₂ photoanode to enhance the performance of dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2017 , 136, 97-103	4.6	21
134	Single transition metal atoms on nitrogen-doped carbon for CO ₂ electrocatalytic reduction: CO production or further CO reduction?. <i>Applied Surface Science</i> , 2020 , 533, 147466	6.7	21
133	Fe/Fe C Boosts H ₂ O Utilization for Methane Conversion Overwhelming O ₂ Generation. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8889-8895	16.4	21
132	Ethanol decomposition on a Pd(110) surface: a density functional theory investigation. <i>Dalton Transactions</i> , 2013 , 42, 2309-18	4.3	20

131	Initial reduction of CO ₂ on perfect and O-defective CeO ₂ (111) surfaces: towards CO or COOH?. <i>RSC Advances</i> , 2015 , 5, 97528-97535	3.7	20
130	Initial hydrogenations of pyridine on MoP(001): a density functional study. <i>Langmuir</i> , 2012 , 28, 3129-37	4	20
129	Rational design of TiO ₂ @ nitrogen-doped carbon coaxial nanotubes as anode for advanced lithium ion batteries. <i>Applied Surface Science</i> , 2018 , 458, 1018-1025	6.7	18
128	A "pre-constrained Metal twins" Strategy to Prepare Efficient dual-metal atom Catalysts for Cooperative Oxygen Electrocatalysis. <i>Advanced Materials</i> , 2021 , e2107421	24	18
127	Theoretical Survey of the Thiophene Hydrodesulfurization Mechanism on Clean and Single-Sulfur-Atom-Modified MoP(001). <i>Journal of Physical Chemistry C</i> , 2016 , 120, 23009-23023	3.8	18
126	CO tolerance of a Pt ₃ Sn(111) catalyst in ethanol decomposition. <i>Catalysis Science and Technology</i> , 2015 , 5, 3246-3258	5.5	17
125	Stimulus-responsive adsorbent materials for CO ₂ capture and separation. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 10519-10533	13	17
124	Direct tuning of meso-/micro-porous structure of carbon nanofibers confining Sb nanocrystals for advanced sodium and potassium storage. <i>Journal of Alloys and Compounds</i> , 2020 , 833, 155127	5.7	17
123	Alkyl amine functionalized triphenylamine-based covalent organic frameworks for high-efficiency CO ₂ capture and separation over N ₂ . <i>Materials Letters</i> , 2018 , 230, 28-31	3.3	17
122	Decomposition of methanethiol on Pt(111): a density functional investigation. <i>Langmuir</i> , 2010 , 26, 12017-25	4.5	17
121	Decomposition mechanism of methylamine to hydrogen cyanide on Pt(111): selectivity of the C-H, N-H and C-N bond scissions. <i>RSC Advances</i> , 2014 , 4, 12266	3.7	16
120	The oxidation pathways of Ti ⁺ by acetaldehyde in the gas phase: A density functional theory investigation. <i>Chemical Physics Letters</i> , 2006 , 431, 56-61	2.5	16
119	Competitive adsorption of CO ₂ /CH ₄ in porous boron nitride nanomaterials. <i>Materials Letters</i> , 2015 , 161, 545-548	3.3	15
118	1, 3-Indanedione functionalized fluorene luminophores: Negative solvatochromism, nanostructure-morphology determined AIE and mechanoresponsive luminescence turn-on. <i>Dyes and Pigments</i> , 2018 , 155, 225-232	4.6	15
117	Effect of alloying on the stabilities and catalytic properties of Ag ₂ Au bimetallic subnanoclusters: a theoretical investigation. <i>Journal of Materials Science</i> , 2016 , 51, 5046-5060	4.3	15
116	Nanoporous Boron Nitride Membranes for Helium Separation. <i>ACS Applied Nano Materials</i> , 2019 , 2, 4471-4479	15	15
115	Theoretical design of push-pull porphyrin dyes with Ebridge modification for dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017 , 332, 232-240	4.7	15
114	Linear thiophene-containing E conjugated aldehydes with aggregation-induced emission for building solid red luminophors. <i>Dyes and Pigments</i> , 2015 , 115, 166-171	4.6	15

113	Gas-phase reactions of Co ⁺ with ethylamine: a theoretical approach to the reaction mechanisms of transition metal ions with primary amines. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 5312-21	2.8	15
112	Can N, S Cocomplexation Promote Single Atom Catalyst Performance in CO RR? Fe-N S Porphyrin versus Fe-N Porphyrin. <i>Small</i> , 2021 , 17, e2100949	11	15
111	Sandwiched Cathodes Assembled from CoS -Modified Carbon Clothes for High-Performance Lithium-Sulfur Batteries. <i>Advanced Science</i> , 2021 , 8, e2101019	13.6	15
110	Li-modified nanoporous carbons for high-performance adsorption and separation of CO ₂ over N ₂ : A combined DFT and GCMC computational study. <i>Journal of CO₂ Utilization</i> , 2018 , 26, 588-594	7.6	14
109	Theoretical analysis of the conversion mechanism of acetylene to ethynylidyne on Pt(111). <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5642-50	3.6	14
108	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. <i>Organic Electronics</i> , 2016 , 29, 142-150	3.5	13
107	Methanol oxidation on Ru(0001) for direct methanol fuel cells: analysis of the competitive reaction mechanism. <i>RSC Advances</i> , 2016 , 6, 1729-1737	3.7	13
106	Theoretical insight into the desulfurization of thiophene on Pt(110): A density functional investigation. <i>Journal of Molecular Catalysis A</i> , 2012 , 363-364, 18-25		13
105	Theoretical investigation on the hydrogen evolution reaction mechanism at MoS ₂ heterostructures: the essential role of the 1T/2H phase interface. <i>Catalysis Science and Technology</i> , 2020 , 10, 458-465	5.5	13
104	Strain-controlled carbon nitride: A continuously tunable membrane for gas separation. <i>Applied Surface Science</i> , 2020 , 506, 144675	6.7	13
103	Diffusion and separation of CH ₄ /N ₂ in pillared graphene nanomaterials: A molecular dynamics investigation. <i>Chemical Physics Letters</i> , 2016 , 660, 272-276	2.5	12
102	Template-directed synthesis of Co ₂ P/MoSe ₂ in a N-doped carbon hollow structure for efficient and stable sodium/potassium ion storage. <i>Nano Energy</i> , 2022 , 93, 106897	17.1	12
101	Carbon Quantum Dots Promote Coupled Valence Engineering of V O Nanobelts for High-Performance Aqueous Zinc-Ion Batteries. <i>ChemSusChem</i> , 2021 , 14, 2076-2083	8.3	12
100	CO ₂ capture and separation over N ₂ and CH ₄ in nanoporous MFM-300(In, Al, Ga, and In-3N): Insight from GCMC simulations. <i>Journal of CO₂ Utilization</i> , 2018 , 28, 145-151	7.6	12
99	Regulation of dithiafulvene-based molecular shape and aggregation on TiO ₂ for high efficiency dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 1974-1981	7.1	11
98	Analysis of Petroleum Aromatics by Laser-Induced Acoustic Desorption/Tunable Synchrotron Vacuum Ultraviolet Photoionization Mass Spectrometry. <i>Energy & Fuels</i> , 2013 , 27, 2010-2017	4.1	11
97	Effects of core moiety and substituted positions in phenothiazine-based hole transporting materials towards high thermal stability and good hole mobility. <i>Tetrahedron</i> , 2017 , 73, 7115-7121	2.4	11
96	First-row transition-metal-doped graphyne for ultrahigh-performance CO ₂ capture and separation over N ₂ /CH ₄ /H ₂ . <i>Materials Today Physics</i> , 2021 , 16, 100301	8	11

95	Carbon phosphides: promising electric field controllable nanoporous materials for CO ₂ capture and separation. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 9970-9980	13	10
94	Theoretical insight into electronic structure and optoelectronic properties of heteroleptic Cu(I)-based complexes for dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2016 , 173, 139-145	4.4	10
93	Mechanistic Insight into Catalytic Oxidation of Ammonia on Clean, O- and OH-Assisted Ir(1 1 1) Surfaces. <i>ChemCatChem</i> , 2013 , 5, 1832-1841	5.2	10
92	Novel heteroatom sulfur porphyrin organic polymer as a metal-free electrocatalyst for acidic oxygen reduction reaction. <i>Electrochimica Acta</i> , 2021 , 377, 138107	6.7	10
91	Dithiafulvene-based organic sensitizers using pyridine as the acceptor for dye-sensitized solar cells. <i>Materials Chemistry and Physics</i> , 2017 , 192, 349-355	4.4	9
90	Hydrodenitrogenation of pyridine on MoP(010): Competition between hydrogenation and denitrification. <i>Inorganica Chimica Acta</i> , 2015 , 435, 30-37	2.7	9
89	In Situ Coupling Reconstruction of Cobalt/Iron Oxide on a Cobalt Phosphate Nanoarray with Interfacial Electronic Features for Highly Enhanced Water Oxidation Catalysis. <i>ACS Sustainable Chemistry and Engineering</i> , 2020 , 8, 4773-4780	8.3	9
88	Blacking of nano-CdS thin film from gas/liquid interface for enhanced photoelectrochemical performances. <i>Applied Surface Science</i> , 2014 , 313, 26-30	6.7	9
87	On the gas-phase Co(+)-mediated oxidation of ethane by N ₂ O: a mechanistic study. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3282-9	2.8	9
86	The competitive O-H versus C-H bond activation of ethanol and methanol by VO ₂ (+) in gas phase: a DFT study. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5161-70	2.8	9
85	Theoretical characterization of ruthenium complexes containing functionalized bithiophene ligands for dye-sensitized solar cells. <i>Journal of Organometallic Chemistry</i> , 2011 , 696, 1632-1639	2.3	9
84	Micelles of Mesoporous Silica with Inserted Iron Complexes as a Platform for Constructing Efficient Electrocatalysts for Oxygen Reduction. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 54720-54731	9.5	9
83	Efficient platinum harvesting of MOF-derived N-doped carbon through cathodic cyclic voltammetry for hydrogen evolution. <i>Electrochimica Acta</i> , 2019 , 317, 173-181	6.7	8
82	Theoretical study of T shaped phenothiazine/carbazole based organic dyes with naphthalimide as spacer for DSSCs. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 233, 118201	4.4	8
81	Theoretical study of the gas-phase Fe ⁺ -mediated oxidation of ethane by N ₂ O. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 349-358	1.9	8
80	Hydride abstraction of methylamine with Cu ⁺ (1S) in the gas phase: A density functional theory study. <i>Journal of Organometallic Chemistry</i> , 2007 , 692, 3796-3803	2.3	8
79	An active site pre-anchoring and post-exposure strategy in Fe(CN) ₆ @PPy derived Fe/S/N-doped carbon electrocatalyst for high performance oxygen reduction reaction and zinc-air batteries. <i>Chemical Engineering Journal</i> , 2021 , 413, 127395	14.7	8
78	The decisive effect of interface states on the photocatalytic activity of the silver(I) oxide/titanium dioxide heterojunction. <i>Journal of Colloid and Interface Science</i> , 2017 , 492, 167-175	9.3	7

77	Enhancing the intermolecular singlet fission efficiency by controlling the self-assembly of amphiphatic tetracene derivatives in aqueous solution. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 11090-11098	7.1	7
76	Unraveling the Mechanism of the Zn-Improved Catalytic Activity of Pd-Based Catalysts for Water-Gas Shift Reaction. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 20181-20191	3.8	7
75	Cu(I)-Based Sensitizers Featuring 6,6'-Dimethyl-4,4'-Dicarboxylate-2,2'-Bipyridine with Functionalized 2,9-Dimethyl-1,10-Phenanthroline Ligands: A Structural, Electronic and Spectral Investigation. <i>Science of Advanced Materials</i> , 2015 , 7, 1361-1367	2.3	7
74	Fe/Fe ₃ C Boosts H ₂ O ₂ Utilization for Methane Conversion Overwhelming O ₂ Generation. <i>Angewandte Chemie</i> , 2021 , 133, 8971-8977	3.6	7
73	Impact of diverse active sites on MoS ₂ catalyst: Competition on active site formation and selectivity of thiophene hydrodesulfurization reaction. <i>Molecular Catalysis</i> , 2019 , 463, 67-76	3.3	7
72	Trivacancy and Stone-Wales defected silicene for adsorption of small gas molecules. <i>Computational Materials Science</i> , 2018 , 154, 276-283	3.2	7
71	Cu acting as Fe activity promoter in dual-atom Cu/Fe-NC catalyst in CO ₂ RR to C ₁ products. <i>Applied Surface Science</i> , 2021 , 564, 150423	6.7	7
70	The properties of the bonding between CO and ZIF-8 structures: a density functional theory study. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	6
69	Ab initio study of hydride abstraction reaction in the Mg+NH ₂ CH ₃ complex. <i>Chemical Physics Letters</i> , 2003 , 381, 109-116	2.5	6
68	Experimental and computational studies of intracomplex reactions in Mg+(primary, secondary alkylamine) complexes induced by photoexcitation of Mg+. <i>Chemistry - A European Journal</i> , 2005 , 11, 6392-406	4.8	6
67	Theoretical Investigation on Novel Porphyrin Dyes with Functionalized Bridge and Donor Groups for Dye-Sensitized Solar Cells. <i>Science of Advanced Materials</i> , 2014 , 6, 2595-2602	2.3	6
66	Oxygen-Doped VS ₄ Microspheres with Abundant Sulfur Vacancies as a Superior Electrocatalyst for the Hydrogen Evolution Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , 2020 , 8, 15055-15064	8.3	6
65	Effects of subnanometer silver clusters on the AgBr(110) photocatalyst surface: a theoretical investigation. <i>Catalysis Science and Technology</i> , 2015 , 5, 4821-4829	5.5	5
64	Theoretical Investigation on Copper(I) Complexes Featuring a Phosphonic Acid Anchor with Asymmetric Ligands for DSSC. <i>ACS Applied Electronic Materials</i> , 2020 , 2, 2141-2150	4	5
63	Density functional theory study of hydrogenation of S to H ₂ S on PtPd alloy surfaces. <i>RSC Advances</i> , 2016 , 6, 6289-6299	3.7	5
62	A Extended tetrathiafulvene derivative: Synthesis and photoluminescence properties. <i>Materials Chemistry and Physics</i> , 2014 , 146, 193-197	4.4	5
61	Preparation of large diameter and low density ZnS microtube arrays via a sacrificial template method. <i>Materials Letters</i> , 2014 , 115, 140-143	3.3	5
60	Theoretical insight into the spectral characteristics of Fe(II)-based complexes for dye-sensitized solar cells: Functionalized bipyridyl chromophores. <i>Journal of Organometallic Chemistry</i> , 2013 , 741-742, 168-175	2.3	5

59	Mechanism of C-N Bond Cleavage in Aniline on MoP(001) Surface. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , 2016 , 32, 465-473	3.8	5
58	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. <i>Molecules</i> , 2020 , 25,	4.8	5
57	High-efficiency CO ₂ capture and separation over N ₂ in penta-graphene pores: insights from GCMC and DFT simulations. <i>Journal of Materials Science</i> , 2020 , 55, 16603-16611	4.3	5
56	Facile control of surface reconstruction with Co ²⁺ or Co ³⁺ -rich (oxy)hydroxide surface on ZnCo phosphate for large-current-density hydrogen evolution in alkali. <i>Materials Today Physics</i> , 2021 , 20, 100448	8.8	5
55	Theoretical insight into photo-induced intramolecular electron transfer in heterodinuclear Ru(II)-Co(III) complexes. <i>Materials Chemistry and Physics</i> , 2015 , 162, 6-10	4.4	4
54	Theoretical analysis of the absorption spectrum, electronic structure, excitation, and intramolecular electron transfer of D-ANEA porphyrin dyes for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 14846-14856	3.6	4
53	Phase transitions of actinium dihydride: Pressure-induced charge transfer driving effect. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 15827-15835	6.7	4
52	Mechanistic insight into the gas-phase reactions of methylamine with ground state Co ⁺ (3F) and Ni ⁺ (2D). <i>Journal of Physical Chemistry A</i> , 2010 , 114, 12490-7	2.8	4
51	Mechanisms for the Ni ⁺ -mediated oxidation of benzene to phenol by N ₂ O. <i>Chemical Physics Letters</i> , 2008 , 463, 54-59	2.5	4
50	Investigation on CH ₃ SH Desulfurization Mechanism at the Edge Site of Co-Doped MoS ₂ Cluster. <i>Acta Chimica Sinica</i> , 2018 , 76, 62	3.3	4
49	Investigation on Oxygen Reduction Reaction Mechanism on S Doped Fe-NC Isolated Single Atoms Catalyst. <i>Acta Chimica Sinica</i> , 2020 , 78, 1001	3.3	4
48	Effect of alloying on the stabilities and catalytic properties of Pt ₂ Au bimetallic subnanoclusters: a theoretical investigation. <i>Journal of Nanoparticle Research</i> , 2016 , 18, 1	2.3	4
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19	Reversing the Photocatalytic Activity Orders of Anatase TiO ₂ Facets by Surface Treatment. <i>ChemistrySelect</i> , 2016, 1, 5838-5841	1.8	1
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17	Single-Atom-like B-N Sites in Ordered Macroporous Carbon for Efficient Oxygen Reduction Reaction. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 53892-53903	9.5	1
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