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	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
2	Ultrahigh Hydrogen Uptake in an Interpenetrated Zn ₄ O-Based Metalâ€“Organic Framework. CCS Chemistry, 2022, 4, 832-837.	7.8	9
3	Synergistic doping and tailoring: Realizing in depth modulation on valence state of CoFe spinel oxide for high-efficiency water oxidation. Applied Surface Science, 2022, 572, 151388.	6.1	4
4	Enabling kinetically fast activation of carbon nanotube@nickel selenide through pore-phase dual regulation in aqueous zinc battery. Science China Materials, 2022, 65, 929-938.	6.3	5
5	Pdâ€“Fe3O4 Janus nanozyme with rational design for ultrasensitive colorimetric detection of biothiols. Biosensors and Bioelectronics, 2022, 196, 113724.	10.1	42
6	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
7	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
8	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
9	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
10	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
11	Composition-Tuned Surface Binding on CuZn-Ni Catalysts Boosts CO₂RR Selectivity toward CO Generation. , 2022, 4, 497-504.		26
12	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
13	Functionalized linker to form high-symmetry adsorption sites in micropore COF for CO2 capture and separation: insight from GCMC simulations. Journal of Materials Science, 2022, 57, 6282-6292.	3.7	8
14	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
15	Precise regulation of CO2 packing pattern in s-block metal doped single-layer covalent organic frameworks for high-performance CO2 capture and separation. Chemical Engineering Journal, 2022, 441, 135903.	12.7	7
16	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
17	Can Chargeâ€Modulated Metalâ€Organic Frameworks Achieve Highâ€Performance CO ₂ Capture and Separation over H ₂ , N ₂ , and CH ₄ ?. ChemSusChem, 2022, 15, .	6.8	8
18	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

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19	Tunable rare-earth metalâ^'organic frameworks for ultra-high selenite capture. Journal of Hazardous Materials, 2022, 436, 129094.	12.4	11
20	Phosphate Group Dependent Metallic Co(OH)₂ toward Hydrogen Evolution in Alkali for the Industrial Current Density. ACS Sustainable Chemistry and Engineering, 2022, 10, 7100-7107.	6.7	7
21	Nitrogen Atom-Doped Layered Graphene for High-Performance CO2/N2 Adsorption and Separation. Energies, 2022, 15, 3713.	3.1	5
22	Constructing surface vacancy to activate the stuck MXenes for high-performance CO2 reduction reaction. Journal of CO2 Utilization, 2022, 62, 102074.	6.8	15
23	Theoretical investigation on two-dimensional conjugated aromatic polymer membranes for high-efficiency hydrogen separation: The effects of pore size and interaction. Separation and Purification Technology, 2022, 299, 121674.	7.9	1
24	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
25	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
26	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
27	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
28	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
29	Innentitelbild: Fe/Fe₃C Boosts H₂O₂ Utilization for Methane Conversion Overwhelming O₂ Generation (Angew. Chem. 16/2021). Angewandte Chemie, 2021, 133, 8642-8642.	2.0	0
30	Fe/Fe₃C Boosts H₂O₂ Utilization for Methane Conversion Overwhelming O₂ Generation. Angewandte Chemie, 2021, 133, 8971-8977.	2.0	26
31	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
32	Tracking CO2 capture and separation over N2 in a flexible metalâ€"organic framework: insights from GCMC and DFT simulations. Journal of Materials Science, 2021, 56, 10414-10423.	3.7	8
33	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
34	Fe/Fe₃C Boosts H₂O₂ Utilization for Methane Conversion Overwhelming O₂ Generation. Angewandte Chemie - International Edition, 2021, 60, 8889-8895.	13.8	66
35	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
36	RÃ¼cktitelbild: Oneâ€step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobaltâ€Functionalized Metalâ€"Organic Frameworks (Angew. Chem. 20/2021). Angewandte Chemie, 2021, 133, 11636-11636.	2.0	0

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37	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
38	Novel heteroatom sulfur porphyrin organic polymer as a metal-free electrocatalyst for acidic oxygen reduction reaction. Electrochimica Acta, 2021, 377, 138107.	5.2	26
39	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
40	Sandwiched Cathodes Assembled from CoS₂â€Modified Carbon Clothes for Highâ€Performance Lithiumâ€Sulfur Batteries. Advanced Science, 2021, 8, e2101019.	11.2	64
41	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
42	Strain-controlled DHP-graphene for ultrahigh-performance hydrogen purification. Applied Surface Science, 2021, 553, 149575.	6.1	3
43	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
44	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
45	Multi-objective optimization of alkali/alkaline earth metals doped graphyne for ultrahigh-performance CO2 capture and separation over N2/CH4. Materials Today Physics, 2021, 21, 100539.	6.0	4
46	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
47	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
48	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
49	Theoretical Investigation of the Fusion Process of Mono-Cages to Tri-Cages with CH4/C2H6 Guest Molecules in sI Hydrates. Molecules, 2021, 26, 7071.	3.8	0
50	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
51	Theoretical Investigation on Denitrification Mechanism of Piperidine: Effects of Methylation Versus Protonation on Câ€“N Bond Activation. Catalysis Letters, 2020, 150, 631-639.	2.6	1
52	Penta-graphene as a promising controllable CO2 capture and separation material in an electric field. Applied Surface Science, 2020, 502, 144067.	6.1	49
53	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
54	Strain-controlled carbon nitride: A continuously tunable membrane for gas separation. Applied Surface Science, 2020, 506, 144675.	6.1	29

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55	Unraveling the Active Site and Mechanism for Câ€“S Bond Activation in Alumina-Supported Pt Catalysts: Ab Initio Insights into Catalytic Desulfurization. Journal of Physical Chemistry C, 2020, 124, 446-458.	3.1	4
56	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
57	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
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. Molecules, 2020, 25, 3681.	3.8	16
59	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
60	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
61	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
62	Theoretical analysis of the absorption spectrum, electronic structure, excitation, and intramolecular electron transfer of Dâ€“Aâ€²â€“Ï€â€“A porphyrin dyes for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2020, 22, 14846-14856.	2.8	8
63	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
64	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
65	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
66	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
67	Stimulus-responsive adsorbent materials for CO₂ capture and separation. Journal of Materials Chemistry A, 2020, 8, 10519-10533.	10.3	39
68	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
69	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
70	Investigation on Oxygen Reduction Reaction Mechanism on S Doped Fe-NC Isolated Single Atoms Catalyst. Acta Chimica Sinica, 2020, 78, 1001.	1.4	7
71	Mechanisms into Hydrogen Purification in a Graphene-like Carbon Nitride Separation Membrane. Wuji Cailiao Xuebao/Journal of Inorganic Materials, 2020, , 655.	1.3	0
72	Initiating an efficient electrocatalyst for water splitting via valence configuration of cobalt-iron oxide. Applied Catalysis B: Environmental, 2019, 258, 117968.	20.2	70

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73	Nanoporous Boron Nitride Membranes for Helium Separation. ACS Applied Nano Materials, 2019, 2, 4471-4479.	5.0	25
74	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
75	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
76	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
77	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
78	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
79	In Situ Growth of MOF-Derived NaCoPO₄@Carbon for Asymmetric Supercapacitive and Water Oxidation Electrocatalytic Performance. Nano, 2019, 14, 1950148.	1.0	7
80	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
81	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
82	Mechanistic insights into porous graphene membranes for helium separation and hydrogen purification. Applied Surface Science, 2018, 441, 631-638.	6.1	42
83	Synthesis and Properties of Dithiafulvenyl Functionalized Spiro[fluorene-9,9â€²-xanthene] Molecules. Organic Letters, 2018, 20, 780-783.	4.6	28
84	A facile co-precipitation synthesis of robust FeCo phosphate electrocatalysts for efficient oxygen evolution. Electrochimica Acta, 2018, 264, 244-250.	5.2	36
85	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
86	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
87	Trivacancy and Stone-Wales defected silicene for adsorption of small gas molecules. Computational Materials Science, 2018, 154, 276-283.	3.0	8
88	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
89	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
90	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

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91	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
92	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
93	Investigation on CH3SH Desulfurization Mechanism at the Edge Site of Co-Doped MoS2 Cluster. Acta Chimica Sinica, 2018, 76, 62.	1.4	4
94	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
95	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
96	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
97	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
98	Edge-functionalized nanoporous carbons for high adsorption capacity and selectivity of CO2 over N2. Applied Surface Science, 2017, 410, 259-266.	6.1	25
99	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
100	Achieving red/near-infrared mechanoresponsive luminescence turn-on: mechanically disturbed metastable nanostructures in organic solids. Chemical Communications, 2017, 53, 1309-1312.	4.1	45
101	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
102	Enhancing Selective Photooxidation through Coâ€“Nx-doped Carbon Materials as Singlet Oxygen Photosensitizers. ACS Catalysis, 2017, 7, 7267-7273.	11.2	111
103	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
104	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
105	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
106	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
107	Effect of alloying on the stabilities and catalytic properties of Ptâ€“Au bimetallic subnanoclusters: a theoretical investigation. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	5
108	Methanol Oxidation on Pt₃Sn(111) for Direct Methanol Fuel Cells: Methanol Decomposition. ACS Applied Materials & Interfaces, 2016, 8, 12194-12204.	8.0	52

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109	Molecular dynamics simulation of fluid properties by the streamwise oscillation of the solid wall. Molecular Simulation, 2016, 42, 1535-1540.	2.0	0
110	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
111	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
112	Role of functionalized acceptors in heteroleptic bipyridyl Cu(I) complexes for dye-sensitized solar cells. Electronic Materials Letters, 2016, 12, 589-595.	2.2	1
113	Diffusion and separation of CH4/N2 in pillared graphene nanomaterials: A molecular dynamics investigation. Chemical Physics Letters, 2016, 660, 272-276.	2.6	17
114	First-principles insight into the photoelectronic properties of Ge-based perovskites. RSC Advances, 2016, 6, 86976-86981.	3.6	51
115	Reversing the Photocatalytic Activity Orders of Anatase TiO₂ Facets by Surface Treatment. ChemistrySelect, 2016, 1, 5838-5841.	1.5	1
116	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
117	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
118	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
119	Density functional theory study of hydrogenation of S to H₂S on Ptâ€“Pd alloy surfaces. RSC Advances, 2016, 6, 6289-6299.	3.6	6
120	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
121	Mechanism of Câ€•N Bond Cleavage in Aniline on MoP(001) Surface. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 465-473.	4.9	7
122	First-Principles Investigation of the Structural and Photoelectronic Properties of CH₃NH₃Pb_{<i>x</i>}Sn<sub>1−<i>x</i&g Mixed Perovskites. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 1439-1445.	4.9	4
123	First-Principles Theory Investigation on Structural and Photoelectronic Properties of Perovskites:Trigonal versus Hexagonal HC(NH2)2PbI3. Acta Chimica Sinica, 2016, 74, 1003.	1.4	1
124	First-Principles Theory Investigation on Structural and Photoelectronic Properties of Formamidinium Lead Halide Perovskites. Acta Chimica Sinica, 2016, 74, 689.	1.4	0
125	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
126	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

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127	The ligand effect on the selective Câ€“H versus Câ€“C bond activation of propane by NiBr+: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	0
128	Effects of subnanometer silver clusters on the AgBr(110) photocatalyst surface: a theoretical investigation. Catalysis Science and Technology, 2015, 5, 4821-4829.	4.1	7
129	Theoretical insight into photo-induced intramolecular electron transfer in heterodinuclear Ru(II)â€“Co(III) complexes. Materials Chemistry and Physics, 2015, 162, 6-10.	4.0	5
130	Hydrodenitrogenation of pyridine on MoP(010): Competition between hydrogenation and denitrification. Inorganica Chimica Acta, 2015, 435, 30-37.	2.4	11
131	Blacking FTO by strongly cathodic polarization with enhanced photocurrent. Applied Surface Science, 2015, 347, 321-324.	6.1	2
132	CO tolerance of a Pt₃Sn(111) catalyst in ethanol decomposition. Catalysis Science and Technology, 2015, 5, 3246-3258.	4.1	17
133	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
134	Strategies to enhance CO₂capture and separation based on engineering absorbent materials. Journal of Materials Chemistry A, 2015, 3, 12118-12132.	10.3	98
135	Competitive adsorption of CO2/CH4 in porous boron nitride nanomaterials. Materials Letters, 2015, 161, 545-548.	2.6	17
136	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
137	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
138	Competitive adsorption of a binary CO₂â€“CH₄ mixture in nanoporous carbons: effects of edge-functionalization. Nanoscale, 2015, 7, 1002-1012.	5.6	145
139	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
140	Theoretical Insight into Organic Dyes Incorporating Triphenylamine-Based Donors and Binary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M1"><mml:mrow><mml:mi mathvariant="bold-italic">Ï€</mml:mi></mml:mrow></mml:math>-Conjugated Bridges for Dye-Sensitized Solar Cells. International Journal of Photoenergy, 2014, 2014, 1-9.	2.5	3
141	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
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