Xiaoqing Lu

List of Publications by Year in Descending Order

184 papers	3,093 citations	31 h-index	45 g-index
195 ext. papers	4,051 ext. citations	6.2 avg, IF	5.42 L-index

#	Paper	IF	Citations
184	Hydrothermal synthesis of ammonium vanadate [(NH4)2V7O16·3.6H2O] as a promising zinc-ion cathode: Experimental and theoretical study of its storage. *Electrochimica Acta*, **2022**, 404, 139785	6.7	2
183	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	17.1	12
182	Pd-FeO Janus nanozyme with rational design for ultrasensitive colorimetric detection of biothiols. *Biosensors and Bioelectronics*, **2022**, 196, 113724	11.8	2
181	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	4.3	1
180	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	14.7	1
179	Surface self-reconstruction of telluride induced by in-situ cathodic electrochemical activation for enhanced water oxidation performance. *Applied Catalysis B: Environmental*, **2022**, 310, 121355	21.8	2
178	Theoretical investigation on electrocatalytic reduction of CO2 to methanol and methane by bimetallic atoms TM1/TM2-N@Gra (TM□Fe, Co, Ni, Cu). *Applied Surface Science*, **2022**, 593, 153377	6.7	0
177	Tunable rare-earth metal-organic frameworks for ultra-high selenite capture.. *Journal of Hazardous Materials*, **2022**, 436, 129094	12.8	1
176	Nitrogen Atom-Doped Layered Graphene for High-Performance CO2/N2 Adsorption and Separation. *Energies*, **2022**, 15, 3713	3.1	
175	Single-Atom-like B-N Sites in Ordered Macroporous Carbon for Efficient Oxygen Reduction Reaction. *ACS Applied Materials & Interfaces*, **2021**, 13, 53892-53903	9.5	1
174	Boosting oxygen evolution reaction of hierarchical spongy NiFe-PBA/Ni3C(B) electrocatalyst: Interfacial engineering with matchable structure. *Chemical Engineering Journal*, **2021**, 433, 133524	14.7	3
173	Triple-atom catalysts 3TM-GYs (TM□Cu, Fe, and Co; GY□graphyne) for high-performance CO2 reduction reaction to C1 products. *Applied Materials Today*, **2021**, 25, 101245	6.6	0
172	A "pre-constrained Metal twins" Strategy to Prepare Efficient dual-metal atom Catalysts for Cooperative Oxygen Electrocatalysis. *Advanced Materials*, **2021**, e2107421	24	18
171	Conversion of Amorphous MOF Microspheres into a Nickel Phosphate Battery-Type Electrode Using the "Anticollapse" Two-Step Strategy. *Inorganic Chemistry*, **2021**, 60, 17094-17102	5.1	3
170	Fe/Fe3C Boosts H2O2 Utilization for Methane Conversion Overwhelming O2 Generation. *Angewandte Chemie*, **2021**, 133, 8971-8977	3.6	7
169	Carbon Quantum Dots Promote Coupled Valence Engineering of V O Nanobelts for High-Performance Aqueous Zinc-Ion Batteries. *ChemSusChem*, **2021**, 14, 2076-2083	8.3	12
168	Tracking CO2 capture and separation over N2 in a flexible metal□organic framework: insights from GCMC and DFT simulations. *Journal of Materials Science*, **2021**, 56, 10414-10423	4.3	1

167	One-step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobalt-Functionalized Metal□Organic Frameworks. *Angewandte Chemie*, **2021**, 133, 11451-11459	3.6	2
166	Fe/Fe C Boosts H O Utilization for Methane Conversion Overwhelming O Generation. *Angewandte Chemie - International Edition*, **2021**, 60, 8889-8895	16.4	21
165	Promotion of electrochemical CO2 reduction to ethylene on phosphorus-doped copper nanocrystals with stable Cu□ sites. *Applied Surface Science*, **2021**, 544, 148965	6.7	3
164	R□cktitelbild: One-step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobalt-Functionalized Metal□Organic Frameworks (Angew. Chem. 20/2021). *Angewandte Chemie*, **2021**, 133, 11636-11636	3.6	
163	Rational Design and Effective Control of Gold-Based Bimetallic Electrocatalyst for Boosting CO Reduction Reaction: A First-Principles Study. *ChemSusChem*, **2021**, 14, 2731-2739	8.3	2
162	Novel heteroatom sulfur porphyrin organic polymer as a metal-free electrocatalyst for acidic oxygen reduction reaction. *Electrochimica Acta*, **2021**, 377, 138107	6.7	10
161	Can N, S Cocoordination Promote Single Atom Catalyst Performance in CO RR? Fe-N S Porphyrin versus Fe-N Porphyrin. *Small*, **2021**, 17, e2100949	11	15
160	Sandwiched Cathodes Assembled from CoS -Modified Carbon Clothes for High-Performance Lithium-Sulfur Batteries. *Advanced Science*, **2021**, 8, e2101019	13.6	15
159	Interfacial Mo-N-C Bond Endowed Hydrogen Evolution Reaction on MoSe@N-Doped Carbon Hollow Nanoflowers. *Inorganic Chemistry*, **2021**, 60, 12377-12385	5.1	2
158	Strain-controlled DHP-graphene for ultrahigh-performance hydrogen purification. *Applied Surface Science*, **2021**, 553, 149575	6.7	1
157	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	14.7	8
156	First-row transition-metal-doped graphyne for ultrahigh-performance CO2 capture and separation over N2/CH4/H2. *Materials Today Physics*, **2021**, 16, 100301	8	11
155	Contemporaneous inverse manipulation of the valence configuration to preferred Co2+ and Ni3+ for enhanced overall water electrocatalysis. *Applied Catalysis B: Environmental*, **2021**, 284, 119725	21.8	23
154	One-step Ethylene Purification from an Acetylene/Ethylene/Ethane Ternary Mixture by Cyclopentadiene Cobalt-Functionalized Metal-Organic Frameworks. *Angewandte Chemie - International Edition*, **2021**, 60, 11350-11358	16.4	24
153	Innentitelbild: Fe/Fe3C Boosts H2O2 Utilization for Methane Conversion Overwhelming O2 Generation (Angew. Chem. 16/2021). *Angewandte Chemie*, **2021**, 133, 8642-8642	3.6	
152	Synergistic doping and tailoring: Realizing in depth modulation on valence state of CoFe spinel oxide for high-efficiency water oxidation. *Applied Surface Science*, **2021**, 572, 151388	6.7	2
151	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	8	5
150	Cu acting as Fe activity promoter in dual-atom Cu/Fe-NC catalyst in CO2RR to C1 products. *Applied Surface Science*, **2021**, 564, 150423	6.7	7

149	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	8	1
148	Metastable marcasite NiSe nanodendrites on carbon fiber clothes to suppress polysulfide shuttling for high-performance lithium-sulfur batteries. *Nanoscale*, **2021**, 13, 16487-16498	7.7	2
147	Can charge-modulated metal-organic frameworks achieve high-performance CO2 capture and separation over H2, N2 and CH4?. *ChemSusChem*, **2021**,	8.3	2
146	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	5
145	Theoretical analysis of the absorption spectrum, electronic structure, excitation, and intramolecular electron transfer of D-A□A porphyrin dyes for dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2020**, 22, 14846-14856	3.6	4
144	In Situ Coupling Reconstruction of Cobalt□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	8.3	9
143	Theoretical study of T shaped phenothiazine/carbazole based organic dyes with naphthalimide as □spacer for DSSCs. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 233, 118201	4.4	8
142	Carbon phosphides: promising electric field controllable nanoporous materials for CO2 capture and separation. *Journal of Materials Chemistry A*, **2020**, 8, 9970-9980	13	10
141	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	21.8	60
140	Stimulus-responsive adsorbent materials for CO2 capture and separation. *Journal of Materials Chemistry A*, **2020**, 8, 10519-10533	13	17
139	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	5.7	17
138	Investigation on Oxygen Reduction Reaction Mechanism on S Doped Fe-NC Isolated Single Atoms Catalyst. *Acta Chimica Sinica*, **2020**, 78, 1001	3.3	4
137	Tuning singlet fission in amphipathic tetracene nanoparticles by controlling the molecular packing with side-group engineering. *Materials Chemistry Frontiers*, **2020**, 4, 2113-2125	7.8	3
136	Penta-graphene as a promising controllable CO2 capture and separation material in an electric field. *Applied Surface Science*, **2020**, 502, 144067	6.7	32
135	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	5.5	13
134	Strain-controlled carbon nitride: A continuously tunable membrane for gas separation. *Applied Surface Science*, **2020**, 506, 144675	6.7	13
133	Unraveling the Active Site and Mechanism for C□S Bond Activation in Alumina-Supported Pt Catalysts: Ab Initio Insights into Catalytic Desulfurization. *Journal of Physical Chemistry C*, **2020**, 124, 446-458	3.8	0
132	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	9.5	9

131	Single transition metal atoms on nitrogen-doped carbon for CO2 electrocatalytic reduction: CO production or further CO reduction?. *Applied Surface Science*, **2020**, 533, 147466	6.7	21
130	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,	4.8	5
129	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	8.3	6
128	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	4.3	5
127	Theoretical Investigation on Denitrification Mechanism of Piperidine: Effects of Methylation Versus Protonation on C–N Bond Activation. *Catalysis Letters*, **2020**, 150, 631-639	2.8	0
126	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	7.1	7
125	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	7.1	11
124	Efficient platinum harvesting of MOF-derived N-doped carbon through cathodic cyclic voltammetry for hydrogen evolution. *Electrochimica Acta*, **2019**, 317, 173-181	6.7	8
123	Rational Design of Metallic NiTex (x = 1 or 2) as Bifunctional Electrocatalysts for Efficient Urea Conversion. *ACS Applied Energy Materials*, **2019**, 2, 3363-3372	6.1	26
122	Initiating an efficient electrocatalyst for water splitting via valence configuration of cobalt-iron oxide. *Applied Catalysis B: Environmental*, **2019**, 258, 117968	21.8	47
121	Nanoporous Boron Nitride Membranes for Helium Separation. *ACS Applied Nano Materials*, **2019**, 2, 4471-4479	5.4	15
120	Electrochemical CO Reduction to C Products on Single Nickel/Cobalt/Iron-Doped Graphitic Carbon Nitride: A DFT Study. *ChemSusChem*, **2019**, 12, 5126-5132	8.3	35
119	In Situ Growth of MOF-Derived NaCoPO4@Carbon for Asymmetric Supercapacitive and Water Oxidation Electrocatalytic Performance. *Nano*, **2019**, 14, 1950148	1.1	4
118	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	4.4	22
117	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	3.3	7
116	Mechanistic insights into porous graphene membranes for helium separation and hydrogen purification. *Applied Surface Science*, **2018**, 441, 631-638	6.7	31
115	Synthesis and Properties of Dithiafulvenyl Functionalized Spiro[fluorene-9,9′-xanthene] Molecules. *Organic Letters*, **2018**, 20, 780-783	6.2	24
114	A facile co-precipitation synthesis of robust FeCo phosphate electrocatalysts for efficient oxygen evolution. *Electrochimica Acta*, **2018**, 264, 244-250	6.7	26

113	1, 3-Indanedione functionalized fluorene luminophores: Negative solvatochromism, nanostructure-morphology determined AIE and mechanoresponsive luminescence turn-on. *Dyes and Pigments*, **2018**, 155, 225-232	4.6	15
112	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	7.6	14
111	Rational design of TiO2@ nitrogen-doped carbon coaxial nanotubes as anode for advanced lithium ion batteries. *Applied Surface Science*, **2018**, 458, 1018-1025	6.7	18
110	Coupled Heterostructure of Mo-Fe Selenide Nanosheets Supported on Carbon Paper as an Integrated Electrocatalyst for Efficient Hydrogen Evolution. *ACS Applied Materials & Interfaces*, **2018**, 10, 27787-27794	9.5	30
109	Alkyl amine functionalized triphenylamine-based covalent organic frameworks for high-efficiency CO2 capture and separation over N2. *Materials Letters*, **2018**, 230, 28-31	3.3	17
108	Investigation on CH3SH Desulfurization Mechanism at the Edge Site of Co-Doped MoS2 Cluster. *Acta Chimica Sinica*, **2018**, 76, 62	3.3	4
107	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	7.6	12
106	Trivacancy and Stone-Wales defected silicene for adsorption of small gas molecules. *Computational Materials Science*, **2018**, 154, 276-283	3.2	7
105	Design of Palladium-Doped g-C3N4 for Enhanced Photocatalytic Activity toward Hydrogen Evolution Reaction. *ACS Applied Energy Materials*, **2018**, 1, 2866-2873	6.1	48
104	Label-free detection of 3-nitro-l-tyrosine with nickel-doped graphene localized surface plasmon resonance biosensor. *Biosensors and Bioelectronics*, **2017**, 89, 468-476	11.8	35
103	Tetra-carbazole substituted spiro[fluorene-9,9?-xanthene]-based hole-transporting materials with high thermal stability and mobility for efficient OLEDs. *Dyes and Pigments*, **2017**, 139, 764-771	4.6	29
102	Dithiafulvene-based organic sensitizers using pyridine as the acceptor for dye-sensitized solar cells. *Materials Chemistry and Physics*, **2017**, 192, 349-355	4.4	9
101	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	6.7	56
100	Edge-functionalized nanoporous carbons for high adsorption capacity and selectivity of CO2 over N2. *Applied Surface Science*, **2017**, 410, 259-266	6.7	23
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	9.3	7
98	Achieving red/near-infrared mechanoresponsive luminescence turn-on: mechanically disturbed metastable nanostructures in organic solids. *Chemical Communications*, **2017**, 53, 1309-1312	5.8	34
97	Architecting a Mesoporous N-Doped Graphitic Carbon Framework Encapsulating CoTe as an Efficient Oxygen Evolution Electrocatalyst. *ACS Applied Materials & Interfaces*, **2017**, 9, 36146-36153	9.5	44
96	Enhancing Selective Photooxidation through CoNx-doped Carbon Materials as Singlet Oxygen Photosensitizers. *ACS Catalysis*, **2017**, 7, 7267-7273	13.1	55

95	Initial Reduction of CO on Pd-, Ru-, and Cu-Doped CeO(111) Surfaces: Effects of Surface Modification on Catalytic Activity and Selectivity. *ACS Applied Materials & Interfaces*, **2017**, 9, 26107-26117	9.5	49
94	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	2.4	11
93	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	4.6	21
92	Theoretical design of push-pull porphyrin dyes with π-bridge modification for dye-sensitized solar cells. *Journal of Photochemistry and Photobiology A: Chemistry*, **2017**, 332, 232-240	4.7	15
91	Unraveling the Mechanism of the Zn-Improved Catalytic Activity of Pd-Based Catalysts for Water−Gas Shift Reaction. *Journal of Physical Chemistry C*, **2016**, 120, 20181-20191	3.8	7
90	Role of functionalized acceptors in heteroleptic bipyridyl Cu(I) complexes for dye-sensitized solar cells. *Electronic Materials Letters*, **2016**, 12, 589-595	2.9	1
89	Diffusion and separation of CH4/N2 in pillared graphene nanomaterials: A molecular dynamics investigation. *Chemical Physics Letters*, **2016**, 660, 272-276	2.5	12
88	First-principles insight into the photoelectronic properties of Ge-based perovskites. *RSC Advances*, **2016**, 6, 86976-86981	3.7	36
87	Reversing the Photocatalytic Activity Orders of Anatase TiO2 Facets by Surface Treatment. *ChemistrySelect*, **2016**, 1, 5838-5841	1.8	1
86	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	4.4	10
85	Effect of alloying on the stabilities and catalytic properties of Ag–Au bimetallic subnanoclusters: a theoretical investigation. *Journal of Materials Science*, **2016**, 51, 5046-5060	4.3	15
84	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	3.5	13
83	Density functional theory study of hydrogenation of S to H2S on Pt–Pd alloy surfaces. *RSC Advances* , **2016**, 6, 6289-6299	3.7	5
82	Methanol oxidation on Ru(0001) for direct methanol fuel cells: analysis of the competitive reaction mechanism. *RSC Advances*, **2016**, 6, 1729-1737	3.7	13
81	Mechanism of C–N Bond Cleavage in Aniline on MoP(001) Surface. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2016**, 32, 465-473	3.8	5
80	First-Principles Investigation of the Structural and Photoelectronic Properties of CH3NH3PbxSn1-xI3 Mixed Perovskites. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2016**, 32, 1439-1445	3.8	3
79	Effect of alloying on the stabilities and catalytic properties of Pt–Au bimetallic subnanoclusters: a theoretical investigation. *Journal of Nanoparticle Research*, **2016**, 18, 1	2.3	4
78	Methanol Oxidation on Pt3Sn(111) for Direct Methanol Fuel Cells: Methanol Decomposition. *ACS Applied Materials & Interfaces*, **2016**, 8, 12194-204	9.5	47

77	Molecular dynamics simulation of fluid properties by the streamwise oscillation of the solid wall. *Molecular Simulation*, **2016**, 42, 1535-1540	2	
76	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	3.8	18
75	The ligand effect on the selective C□H versus C□C bond activation of propane by NiBr+: a theoretical study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	
74	Effects of subnanometer silver clusters on the AgBr(110) photocatalyst surface: a theoretical investigation. *Catalysis Science and Technology*, **2015**, 5, 4821-4829	5.5	5
73	Theoretical insight into photo-induced intramolecular electron transfer in heterodinuclear Ru(II)□Co(III) complexes. *Materials Chemistry and Physics*, **2015**, 162, 6-10	4.4	4
72	Hydrodenitrogenation of pyridine on MoP(010): Competition between hydrogenation and denitrification. *Inorganica Chimica Acta*, **2015**, 435, 30-37	2.7	9
71	Blacking FTO by strongly cathodic polarization with enhanced photocurrent. *Applied Surface Science*, **2015**, 347, 321-324	6.7	2
70	CO tolerance of a Pt3Sn(111) catalyst in ethanol decomposition. *Catalysis Science and Technology*, **2015**, 5, 3246-3258	5.5	17
69	The properties of the bonding between CO and ZIF-8 structures: a density functional theory study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	6
68	Strategies to enhance CO2 capture and separation based on engineering absorbent materials. *Journal of Materials Chemistry A*, **2015**, 3, 12118-12132	13	87
67	Competitive adsorption of CO2/CH4 in porous boron nitride nanomaterials. *Materials Letters*, **2015**, 161, 545-548	3.3	15
66	The Oxidation of Methanol on PtRu(111): A Periodic Density Functional Theory Investigation. *Journal of Physical Chemistry C*, **2015**, 119, 20389-20400	3.8	35
65	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. *Journal of Materials Chemistry C*, **2015**, 3, 10129-10139	7.1	23
64	Competitive adsorption of a binary CO2-CH4 mixture in nanoporous carbons: effects of edge-functionalization. *Nanoscale*, **2015**, 7, 1002-12	7.7	114
63	Initial reduction of CO2 on perfect and O-defective CeO2 (111) surfaces: towards CO or COOH?. *RSC Advances*, **2015**, 5, 97528-97535	3.7	20
62	Linear thiophene-containing □conjugated aldehydes with aggregation-induced emission for building solid red luminophors. *Dyes and Pigments*, **2015**, 115, 166-171	4.6	15
61	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. *Science of Advanced Materials*, **2015**, 7, 1361-1367	2.3	7
60	A □extended tetrathiafulvene derivative: Synthesis and photoluminescence properties. *Materials Chemistry and Physics*, **2014**, 146, 193-197	4.4	5

59	Preparation of large diameter and low density ZnS microtube arrays via a sacrificial template method. *Materials Letters*, **2014**, 115, 140-143	3.3	5
58	Plasmonic enhanced dye-sensitized solar cells with self-assembly gold-TiO2@core–shell nanoislands. *Solar Energy*, **2014**, 99, 115-125	6.8	35
57	The adsorption behaviour of CH4 on microporous carbons: effects of surface heterogeneity. *Physical Chemistry Chemical Physics*, **2014**, 16, 11037-46	3.6	43
56	Decomposition mechanism of methylamine to hydrogen cyanide on Pt(111): selectivity of the C–H, N–H and C–N bond scissions. *RSC Advances*, **2014**, 4, 12266	3.7	16
55	Phase transitions of actinium dihydride: Pressure-induced charge transfer driving effect. *International Journal of Hydrogen Energy*, **2014**, 39, 15827-15835	6.7	4
54	Effects of atomic Ag on AgBr photocatalyst surfaces: a theoretical survey. *RSC Advances*, **2014**, 4, 33134-33143	3.7	3
53	Blacking of nano-CdS thin film from gas/liquid interface for enhanced photoelectrochemical performances. *Applied Surface Science*, **2014**, 313, 26-30	6.7	9
52	Theoretical Insight into Organic Dyes Incorporating Triphenylamine-Based Donors and Binary–Conjugated Bridges for Dye-Sensitized Solar Cells. *International Journal of Photoenergy*, **2014**, 2014, 1-9	2.1	2
51	Facile fabrication of superhydrophobic Bi/Bi2O3 surfaces with hierarchical micro-nanostructures by electroless deposition or electrodeposition. *Applied Surface Science*, **2014**, 288, 558-563	6.7	31
50	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	6.7	23
49	Theoretical Investigation on Novel Porphyrin Dyes with Functionalized Bridge and Donor Groups for Dye-Sensitized Solar Cells. *Science of Advanced Materials*, **2014**, 6, 2595-2602	2.3	6
48	Ethanol decomposition on a Pd(110) surface: a density functional theory investigation. *Dalton Transactions*, **2013**, 42, 2309-18	4.3	20
47	Theoretical insight into the spectral characteristics of Fe(II)-based complexes for dye-sensitized solar cells: Functionalized bipyridyl chromophores. *Journal of Organometallic Chemistry*, **2013**, 741-742, 168-175	2.3	5
46	Reactivity of ethanol with ground state Ni+(2D) in the gas phase: A density functional study. *Computational and Theoretical Chemistry*, **2013**, 1023, 29-37	2	2
45	Analysis of Petroleum Aromatics by Laser-Induced Acoustic Desorption/Tunable Synchrotron Vacuum Ultraviolet Photoionization Mass Spectrometry. *Energy & Fuels*, **2013**, 27, 2010-2017	4.1	11
44	Photoelectrochemical sensing of Cu2+ ions with SnO2/CdS heterostructural films. *Sensors and Actuators B: Chemical*, **2013**, 183, 601-607	8.5	39
43	Mechanistic Insight into Catalytic Oxidation of Ammonia on Clean, O- and OH-Assisted Ir(1 1 1) Surfaces. *ChemCatChem*, **2013**, 5, 1832-1841	5.2	10
42	The competitive O-H versus C-H bond activation of ethanol and methanol by VO2(+) in gas phase: a DFT study. *Journal of Physical Chemistry A*, **2013**, 117, 5161-70	2.8	9

41	Mechanistic insight into the hydrazine decomposition on Rh(111): effect of reaction intermediate on catalytic activity. *Physical Chemistry Chemical Physics*, **2013**, 15, 16172-82	3.6	39
40	Theoretical analysis of the conversion mechanism of acetylene to ethylidyne on Pt(111). *Physical Chemistry Chemical Physics*, **2012**, 14, 5642-50	3.6	14
39	On the gas-phase Co(+)-mediated oxidation of ethane by N2O: a mechanistic study. *Journal of Physical Chemistry A*, **2012**, 116, 3282-9	2.8	9
38	Initial hydrogenations of pyridine on MoP(001): a density functional study. *Langmuir*, **2012**, 28, 3129-37	4	20
37	Theoretical investigation of the reaction of Mn+ with ethylene oxide. *Journal of Physical Chemistry A*, **2012**, 116, 512-9	2.8	2
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