

Jing-xiang Zhao

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Efficient electrochemical reduction of CO to C2 products on the transition metal and boron co-doped black phosphorene. Chinese Chemical Letters, 2022, 33, 2183-2187.	9.0	26
2	Achieving efficient N2 electrochemical reduction by stabilizing the N2H* intermediate with the frustrated Lewis pairs. Journal of Energy Chemistry, 2022, 66, 628-634.	12.9	13
3	Single Ir atom anchored in pyrrolic-N4 doped graphene as a promising bifunctional electrocatalyst for the ORR/OER: a computational study. Journal of Colloid and Interface Science, 2022, 607, 1005-1013.	9.4	78
4	Intramolecular heterostructured carbon nitride with heptazine-triazine for enhanced photocatalytic hydrogen evolution. Chemical Engineering Journal, 2022, 428, 132579.	12.7	86
5	NIR-driven intracellular photocatalytic oxygen-supply on metallic molybdenum carbide@N-carbon for hypoxic tumor therapy. Journal of Colloid and Interface Science, 2022, 607, 1-15.	9.4	17
6	1 T-MoSe2 monolayer supported single Pd atom as a highly-efficient bifunctional catalyst for ORR/OER. Journal of Colloid and Interface Science, 2022, 605, 155-162.	9.4	55
7	Selective oxidation of methanol to dimethoxymethane over iron and vanadate modified phosphotungstate. Applied Surface Science, 2022, 574, 151516.	6.1	8
8	Two-dimensional Pt2P3 monolayer: A promising bifunctional electrocatalyst with different active sites for hydrogen evolution and CO2 reduction. Chinese Chemical Letters, 2022, 33, 3987-3992.	9.0	16
9	Wet-chemistry hydrogen doped TiO2 with switchable defects control for photocatalytic hydrogen evolution. Matter, 2022, 5, 206-218.	10.0	66
10	Synthesis of cuprous oxide nanoparticles on graphitic carbon nitride and reduced graphene oxide and their catalytic performance toward the reduction of 4-nitrophenol. Journal of Materials Science, 2022, 57, 2424-2435.	3.7	5
11	Revisiting catalytic performance of supported metal dimers for oxygen reduction reaction via magnetic coupling from first principles. , 2022, 1, 100031.		31
12	A metallic Cu₂N monolayer with planar tetracoordinated nitrogen as a promising catalyst for CO₂ electroreduction. Journal of Materials Chemistry A, 2022, 10, 1560-1568.	10.3	13
13	Tuning precise numbers of supported nickel clusters on graphdiyne for efficient CO2 electroreduction toward various multi-carbon products. Journal of Energy Chemistry, 2022, 69, 456-465.	12.9	49
14	Computational screening of single-atom catalysts supported by VS₂ monolayers for electrocatalytic oxygen reduction/evolution reactions. Nanoscale, 2022, 14, 6902-6911.	5.6	30
15	Iron and molybdenum modified phosphotungstates towards selective oxidation of styrene to benzaldehyde. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2022, 642, 128736.	4.7	1
16	Tuning single metal atoms anchored on graphdiyne for highly efficient and selective nitrate electroreduction to ammonia under aqueous environments: A computational study. Applied Surface Science, 2022, 592, 153213.	6.1	27
17	Multi-interface MoS₂/Ni₃S₄/Mo₂S₃ composite as an efficient electrocatalyst for hydrogen evolution reaction over a wide pH range. Dalton Transactions, 2022, 51, 6825-6831.	3.3	4
18	Understanding the CH4 Conversion over Metal Dimers from First Principles. Nanomaterials, 2022, 12, 1518.	4.1	2

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19	Phthalocyanine-supported single-atom catalysts as a promising bifunctional electrocatalyst for ORR/OER: A computational study. <i>ChemPhysMater</i> , 2022, 1, 237-245.	2.8	20
20	Exfoliation of graphitic carbon nitride and homogeneous loading of Cu ₂ O catalyst. <i>Solid State Sciences</i> , 2022, 129, 106915.	3.2	4
21	Supported Cu ₃ clusters on graphitic carbon nitride as an efficient catalyst for CO electroreduction to propene. <i>Journal of Materials Chemistry A</i> , 2022, 10, 14460-14469.	10.3	17
22	MoS ₂ induced hollow Cu ₂ O spheres: Synthesis and efficient catalytic performance in the reduction of 4-nitrophenol by NaBH ₄ . <i>Applied Surface Science</i> , 2021, 539, 148285.	6.1	26
23	Coordination Number Regulation of Molybdenum Single-Atom Nanozyme Peroxidase-like Specificity. <i>CheM</i> , 2021, 7, 436-449.	11.7	216
24	Enhanced catalytic activity of MXene for nitrogen electroreduction reaction by carbon doping. <i>Journal of Colloid and Interface Science</i> , 2021, 588, 1-8.	9.4	29
25	Coordination tunes the activity and selectivity of the nitrogen reduction reaction on single-atom iron catalysts: a computational study. <i>Journal of Materials Chemistry A</i> , 2021, 9, 1240-1251.	10.3	135
26	A Composite Fe ^V /g-C ₃ N ₄ for Liquid-Phase Selective Oxidation of Methanol with O ₂ Oxidant. <i>Catalysis Letters</i> , 2021, 151, 909-919.	2.6	2
27	Vacancy-induced high activity of MoS ₂ monolayers for CO electroreduction: a computational study. <i>Sustainable Energy and Fuels</i> , 2021, 5, 4932-4943.	4.9	4
28	A Ni ₃ -embedded MoS ₂ monolayer as a promising electrocatalyst with high activity for the oxygen evolution reaction: a computational study. <i>Sustainable Energy and Fuels</i> , 2021, 5, 3330-3339.	4.9	7
29	Tuneable oxidation of styrene to benzaldehyde and benzoic acid over Co/ZSM-5. <i>New Journal of Chemistry</i> , 2021, 45, 18192-18201.	2.8	11
30	P- or S-Doped graphdiyne as a superior metal-free electrocatalyst for the hydrogen evolution reaction: a computational study. <i>New Journal of Chemistry</i> , 2021, 45, 8101-8108.	2.8	14
31	Experimental and theoretical investigation of the enhancement of the photo-oxidation of Hg ⁰ by CeO ₂ -modified morphology-controlled anatase TiO ₂ . <i>Journal of Hazardous Materials</i> , 2021, 406, 124535.	12.4	20
32	Stable Bimetallic Hydride Boosts Anodic CO Tolerance of Fuel Cells. <i>ACS Energy Letters</i> , 2021, 6, 1912-1919.	17.4	48
33	2D Bismuthene Metal Electron Mediator Engineering Super Interfacial Charge Transfer for Efficient Photocatalytic Reduction of Carbon Dioxide. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 21582-21592.	8.0	15
34	Fe ₃ O ₄ /g-C ₃ N ₄ -CeO _x fabricated by in situ-reduction towards solvent-free oxidation of styrene to benzaldehyde. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 616, 126309.	4.7	7
35	Copper vanadate nanowires on g-C ₃ N ₄ toward highly selective oxidation of methanol to dimethoxymethane. <i>Applied Surface Science</i> , 2021, 548, 149180.	6.1	9
36	Synthesis of a Co-Sn Alloy-Deposited PTFE Film for Enhanced Solar-Driven Water Evaporation via a Super-Absorbent Polymer-Based Water Pump-Design. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 26879-26890.	8.0	14

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37	Capture and catalytic conversion of lithium polysulfides by metal-doped MoS ₂ monolayers for lithium-sulfur batteries: A computational study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 130, 114715.	2.7	9
38	VO _x -MoO _y single molecular layer modified graphic carbon nitride polymer for enhanced selective styrene oxidation. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, , .	5.8	3
39	Two-dimensional IrN ₂ monolayer: An efficient bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions. <i>Journal of Colloid and Interface Science</i> , 2021, 600, 711-718.	9.4	27
40	Controlled 2H/1T phase transition in MoS ₂ monolayers by a strong interface with M ₂ C MXenes: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20107-20116.	2.8	13
41	A Pt ₃ cluster anchored on a C ₂ N monolayer as an efficient catalyst for electrochemical reduction of nitrobenzene to aniline: a computational study. <i>New Journal of Chemistry</i> , 2021, 45, 21270-21277.	2.8	3
42	Catalytic oxidation of styrene and its reaction mechanism consideration over bimetal modified phosphotungstates. <i>Molecular Catalysis</i> , 2021, 515, 111940.	2.0	5
43	Boosting nitrogen reduction on single Mo atom by tuning its coordination environment. <i>Sustainable Energy and Fuels</i> , 2021, 5, 6488-6497.	4.9	7
44	Two-dimensional Ī-conjugated metal bis(dithiolene) nanosheet: A promising anchoring material for lithium-sulfur batteries. <i>Computational Materials Science</i> , 2020, 171, 109228.	3.0	15
45	N-heterocyclic carbene as a promising metal-free electrocatalyst with high efficiency for nitrogen reduction to ammonia. <i>Journal of Energy Chemistry</i> , 2020, 46, 78-86.	12.9	33
46	Adsorption and catalytic activation of N ₂ molecule on iron dimer supported by different two-dimensional carbon-based substrates: A computational study. <i>Applied Surface Science</i> , 2020, 506, 144943.	6.1	21
47	PtN ₃ -Embedded graphene as an efficient catalyst for electrochemical reduction of nitrobenzene to aniline: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17639-17645.	2.8	11
48	RuN ₂ Monolayer: A Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 54517-54523.	8.0	22
49	Methane Conversion over C ₂ N-Supported Fe ₂ Dimers. <i>Catalysts</i> , 2020, 10, 973.	3.5	1
50	Fe ₃ Cluster Anchored on the C ₂ N Monolayer for Efficient Electrochemical Nitrogen Fixation. <i>Catalysts</i> , 2020, 10, 974.	3.5	15
51	Size-dependent electrocatalytic activity of ORR/OER on palladium nanoclusters anchored on defective MoS ₂ monolayers. <i>New Journal of Chemistry</i> , 2020, 44, 16135-16143.	2.8	15
52	Polyoxometalate-based metal-organic framework-derived bimetallic hybrid materials for upgraded electrochemical reduction of nitrogen. <i>Green Chemistry</i> , 2020, 22, 6157-6169.	9.0	132
53	FeMoO ₄ nanorods for efficient ambient electrochemical nitrogen reduction. <i>Chemical Communications</i> , 2020, 56, 6834-6837.	4.1	36
54	Flexible Pt ₃ Ni-S-Deposited Teflon Membrane with High Surface Mechanical Properties for Efficient Solar-Driven Strong Acidic/Alkaline Water Evaporation. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 27140-27149.	8.0	22

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55	Strain effect on the catalytic activities of B- and B/N-doped black phosphorene for electrochemical conversion of CO to valuable chemicals. <i>Journal of Materials Chemistry A</i> , 2020, 8, 11986-11995.	10.3	31
56	Transformation of ZIF-8 nanoparticles into 3D nitrogen-doped hierarchically porous carbon for Li ⁺ S batteries. <i>RSC Advances</i> , 2020, 10, 17345-17352.	3.6	12
57	Single transition metal atoms anchored on a C ₂ N monolayer as efficient catalysts for hydrazine electrooxidation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 16691-16700.	2.8	12
58	SO ₄ ²⁻ @Fe ³⁺ /ZrO ₂ Composite for Selective Oxidation of Styrene to Benzaldehyde in H ₂ O ₂ Aqueous Solution. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 4411-4418.	3.7	6
59	Tuning the electronic structures of monolayer triphosphides MP ₃ (M = Sn and Ge) for CO ₂ electroreduction through interface engineering: a theoretical prediction. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6896-6905.	2.8	10
60	Graphdiyne-Supported Single Iron Atom: A Promising Electrocatalyst for Carbon Dioxide Electroreduction into Methane and Ethanol. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3722-3730.	3.1	75
61	Boosting ppb-level triethylamine sensing of ZnO: adjusting proportions of electron donor defects. <i>Journal of Materials Chemistry C</i> , 2020, 8, 6734-6742.	5.5	25
62	A Cu ₂ B ₂ monolayer with planar hypercoordinate motifs: an efficient catalyst for CO electroreduction to ethanol. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9607-9615.	10.3	32
63	Optimal Configuration of N-Doped Carbon Defects in 2D Turbostratic Carbon Nanomesh for Advanced Oxygen Reduction Electrocatalysis. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11999-12006.	13.8	121
64	Optimal Configuration of N-Doped Carbon Defects in 2D Turbostratic Carbon Nanomesh for Advanced Oxygen Reduction Electrocatalysis. <i>Angewandte Chemie</i> , 2020, 132, 12097-12104.	2.0	21
65	Nitrogen electroreduction performance of transition metal dimers embedded into N-doped graphene: a theoretical prediction. <i>Journal of Materials Chemistry A</i> , 2020, 8, 4533-4543.	10.3	124
66	Highly Selective Oxidation of Styrene Over FeCl ₃ -Imidazolium Ionic Liquid Grafted SBA-15. <i>Catalysis Letters</i> , 2019, 149, 2994-2999.	2.6	10
67	Ionic Liquid Dispersed Ti/SBA-15 for Double-Bond Cleavage Oxidation of \pm -Methylstyrene into Acetophenone. <i>Catalysis Letters</i> , 2019, 149, 3491-3500.	2.6	6
68	Single Mn atom as a promising electrocatalyst for CO reduction to C ₂ H ₅ OH and C ₃ H ₆ : A computational study. <i>Applied Surface Science</i> , 2019, 498, 143868.	6.1	15
69	B ₄ C ₃ Monolayer with Impressive Electronic, Optical, and Mechanical Properties: A Potential Metal-Free Photocatalyst for CO ₂ Reduction under Visible Light. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25091-25101.	3.1	19
70	Metal-free graphdiyne doped with sp-hybridized boron and nitrogen atoms at acetylenic sites for high-efficiency electroreduction of CO ₂ to CH ₄ and C ₂ H ₄ . <i>Journal of Materials Chemistry A</i> , 2019, 7, 4026-4035.	10.3	87
71	A boron-interstitial doped C ₂ N layer as a metal-free electrocatalyst for N ₂ fixation: a computational study. <i>Journal of Materials Chemistry A</i> , 2019, 7, 2392-2399.	10.3	162
72	Construct of MoSe ₂ /Bi ₂ Se ₃ nanoheterostructure: Multimodal CT/PT imaging-guided PTT/PDT/chemotherapy for cancer treating. <i>Biomaterials</i> , 2019, 217, 119282.	11.4	119

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73	Two-dimensional π -conjugated metal bis(dithiolene) nanosheets as promising electrocatalysts for carbon dioxide reduction: a computational study. <i>Journal of Materials Chemistry A</i> , 2019, 7, 15341-15346.	10.3	40
74	Two-dimensional π -conjugated osmium bis(dithiolene) complex (OsC_4S_4) as a promising electrocatalyst for ambient nitrogen reduction to ammonia. <i>Applied Surface Science</i> , 2019, 487, 833-839.	6.1	39
75	Heterostructures of doped graphene and MoX_2 ($X = \text{S}$ and Se) as promising anchoring materials for lithium-sulfur batteries: a first-principles study. <i>New Journal of Chemistry</i> , 2019, 43, 9396-9402.	2.8	17
76	Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping. <i>Small Methods</i> , 2019, 3, 1800550.	8.6	149
77	Doping MoS_2 monolayer with nonmetal atoms to tune its electronic and magnetic properties, and chemical activity: a computational study. <i>New Journal of Chemistry</i> , 2019, 43, 5766-5772.	2.8	9
78	VO_x molecular level grafted $g\text{-C}_3\text{N}_4$ for highly selective oxidation of methanol to dimethoxymethane. <i>Molecular Catalysis</i> , 2019, 469, 48-56.	2.0	17
79	Elucidating the mechanism of the structure-dependent enzymatic activity of Fe-N/C oxidase mimics. <i>Chemical Communications</i> , 2019, 55, 5271-5274.	4.1	95
80	B-terminated (111) polar surfaces of BP and BAs: promising metal-free electrocatalysts with large reaction regions for nitrogen fixation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 13284-13292.	10.3	87
81	Photodegradation of naphthalene over Fe_3O_4 under visible light irradiation. <i>Royal Society Open Science</i> , 2019, 6, 181779.	2.4	9
82	Frustrated Lewis pairs photocatalyst for visible light-driven reduction of CO to multi-carbon chemicals. <i>Nanoscale</i> , 2019, 11, 20777-20784.	5.6	38
83	Revealing the Intrinsic Peroxidase-Like Catalytic Mechanism of Heterogeneous Single-Atom Co-MoS_2 . <i>Nano-Micro Letters</i> , 2019, 11, 102.	27.0	114
84	Construction of Z-scheme $\text{MoSe}_2/\text{CdSe}$ hollow nanostructure with enhanced full spectrum photocatalytic activity. <i>Applied Catalysis B: Environmental</i> , 2019, 244, 76-86.	20.2	122
85	Electrochemical reduction of carbon dioxide on the two-dimensional $\text{M}_3(\text{Hexaiminotriphenylene})_2$ sheet: A computational study. <i>Applied Surface Science</i> , 2019, 467-468, 98-103.	6.1	45
86	Computational Screening of Efficient Single-Atom Catalysts Based on Graphitic Carbon Nitride ($g\text{-C}_3\text{N}_4$) for Nitrogen Electroreduction. <i>Small Methods</i> , 2019, 3, 1800368.	8.6	347
87	Rational Design of Fe-N/C Hybrid for Enhanced Nitrogen Reduction Electrocatalysis under Ambient Conditions in Aqueous Solution. <i>ACS Catalysis</i> , 2019, 9, 336-344.	11.2	278
88	Single transition metal atom embedded into a MoS_2 nanosheet as a promising catalyst for electrochemical ammonia synthesis. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9248-9255.	2.8	165
89	Computational screening of a single transition metal atom supported on the C_2N monolayer for electrochemical ammonia synthesis. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12835-12844.	2.8	142
90	SiC_2 siligraphene as a promising anchoring material for lithium-sulfur batteries: a computational study. <i>Applied Surface Science</i> , 2018, 440, 889-896.	6.1	32

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91	Nano metal oxides as efficient catalysts for selective synthesis of 1-methoxy-2-propanol from methanol and propylene oxide. RSC Advances, 2018, 8, 4478-4482.	3.6	15
92	A Co ^{II} -N ₄ moiety embedded into graphene as an efficient single-atom-catalyst for NO electrochemical reduction: a computational study. Journal of Materials Chemistry A, 2018, 6, 7547-7556.	10.3	99
93	Metal-N ₄ /graphene as an efficient anchoring material for lithium-sulfur batteries: A computational study. Diamond and Related Materials, 2018, 90, 72-78.	3.9	29
94	Boron-doped graphene as a promising electrocatalyst for NO electrochemical reduction: a computational study. New Journal of Chemistry, 2018, 42, 16346-16353.	2.8	27
95	Negatively charged boron nitride nanosheets as a potential metal-free electrocatalyst for the oxygen reduction reaction: a computational study. New Journal of Chemistry, 2018, 42, 12838-12844.	2.8	12
96	Design and synthesis of surface-controlled CuOx/rGO nanocomposites with unusually high efficiency in catalytic conversion of organic reactants in the presence of NaBH ₄ . Applied Surface Science, 2018, 459, 716-722.	6.1	28
97	Copper Dimer Supported on a C ₂ N Layer as an Efficient Electrocatalyst for CO ₂ Reduction Reaction: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 19712-19721.	3.1	167
98	Highly selective oxidation of styrene to benzaldehyde over Fe ₃ O ₄ using H ₂ O ₂ aqueous solution as oxidant. Reaction Kinetics, Mechanisms and Catalysis, 2018, 125, 743-756.	1.7	18
99	Metal-Organic-Framework-Derived Fe-N/C Electrocatalyst with Five-Coordinated Fe-N Sites for Advanced Oxygen Reduction in Acid Media. ACS Catalysis, 2017, 7, 1655-1663.	11.2	483
100	Computational screening for high-activity MoS ₂ monolayer-based catalysts for the oxygen reduction reaction via substitutional doping with transition metal. Journal of Materials Chemistry A, 2017, 5, 9842-9851.	10.3	81
101	Environmentally benign alcoholysis of urea and disubstituted urea to alkyl carbamates over alkali-treated zeolites. Microporous and Mesoporous Materials, 2017, 248, 108-114.	4.4	10
102	How to make inert boron nitride nanosheets active for the immobilization of polysulfides for lithium-sulfur batteries: a computational study. Physical Chemistry Chemical Physics, 2017, 19, 18208-18216.	2.8	35
103	Component Matters: Paving the Roadmap toward Enhanced Electrocatalytic Performance of Graphitic C ₃ N ₄ -Based Catalysts via Atomic Tuning. ACS Nano, 2017, 11, 6004-6014.	14.6	144
104	An efficient strategy for formation of C-N bond by benzyl chloride over nano Fe ₂ O ₃ . Molecular Catalysis, 2017, 431, 27-31.	2.0	4
105	Functional group-dependent anchoring effect of titanium carbide-based MXenes for lithium-sulfur batteries: A computational study. Applied Surface Science, 2017, 412, 591-598.	6.1	130
106	Frustrated Lewis Pair Catalysts in Two Dimensions: B/Al-Doped Phosphorenes as Promising Catalysts for Hydrogenation of Small Unsaturated Molecules. ACS Catalysis, 2017, 7, 766-771.	11.2	45
107	Small Dopants Make Big Differences: Enhanced Electrocatalytic Performance of MoS ₂ Monolayer for Oxygen Reduction Reaction (ORR) by N and P Doping. Electrochimica Acta, 2017, 225, 543-550.	5.2	106
108	Effect of acidic and red-ox sites over modified ZSM-5 surface on selectivity in oxidation of toluene. Molecular Catalysis, 2017, 442, 20-26.	2.0	12

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109	Highly selective oxidation of methanol to dimethoxymethane over $\text{SO}_4^{2-}/\text{V}_2\text{O}_5/\text{ZrO}_2$. <i>New Journal of Chemistry</i> , 2017, 41, 8370-8376.	2.8	11
110	CO_2 electroreduction performance of a single transition metal atom supported on porphyrin-like graphene: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23113-23121.	2.8	117
111	Single Mo Atom Supported on Defective Boron Nitride Monolayer as an Efficient Electrocatalyst for Nitrogen Fixation: A Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 12480-12487.	13.7	1,006
112	An Efficient Route for Electrooxidation of Methanol to Dimethoxymethane Using Ionic Liquid as Electrolyte. <i>Journal of the Electrochemical Society</i> , 2017, 164, H5074-H5077.	2.9	5
113	Theoretical insights into the energetics and electronic properties of MPt_{12} (M = Fe, Co, Ni, Cu, and Pd) nanoparticles supported by N-doped defective graphene. <i>Applied Surface Science</i> , 2017, 397, 199-205.	6.1	25
114	An organic polymer-grafted ionic liquid as a catalyst for the cycloaddition of CO_2 to epoxides. <i>New Journal of Chemistry</i> , 2017, 41, 387-392.	2.8	15
115	Toward enhanced activity of a graphitic carbon nitride-based electrocatalyst in oxygen reduction and hydrogen evolution reactions via atomic sulfur doping. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12205-12211.	10.3	112
116	A novel strategy for conversion of methanol and CO_2 into dimethoxymethane in a basic ionic liquid. <i>Journal of Molecular Catalysis A</i> , 2016, 421, 117-121.	4.8	17
117	CO oxidation catalyzed by silicon carbide (SiC) monolayer: A theoretical study. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 66, 196-200.	2.4	27
118	Two-dimensional iron tetracyanoquinodimethane (FeTCNQ) monolayer: an efficient electrocatalyst for the oxygen reduction reaction. <i>RSC Advances</i> , 2016, 6, 72952-72958.	3.6	22
119	DFT-based study on the mechanisms of the oxygen reduction reaction on $\text{Co}(\text{acetylacetonate})_2$ supported by N-doped graphene nanoribbon. <i>RSC Advances</i> , 2016, 6, 79662-79667.	3.6	5
120	Pyridine derivative/graphene nanoribbon composites as molecularly tunable heterogeneous electrocatalysts for the oxygen reduction reaction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5040-5047.	2.8	11
121	Single sided fluorine functionalized graphene: A metal free electrocatalyst with high efficiency for oxygen reduction reaction. <i>Carbon</i> , 2016, 104, 56-63.	10.3	51
122	Phosphorene as a promising anchoring material for lithium sulfur batteries: a computational study. <i>Journal of Materials Chemistry A</i> , 2016, 4, 6124-6130.	10.3	156
123	Pyrolic-nitrogen doped graphene: a metal-free electrocatalyst with high efficiency and selectivity for the reduction of carbon dioxide to formic acid: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5491-5498.	2.8	114
124	Ionothermal synthesis and structural characterization of $[\text{Cu}(\text{C}_4\text{H}_6\text{N}_2)_4]\text{Br}_2$ and $[\text{Ni}(\text{C}_4\text{H}_6\text{N}_2)_4]\text{Br}_2$. <i>Journal of Chemical Sciences</i> , 2015, 127, 1261-1265.	1.5	1
125	Mixed Oxides FeVO_x for Selective Oxidation of Octanol to Octanal under Solvent free Condition. <i>Journal of the Chinese Chemical Society</i> , 2015, 62, 722-727.	1.4	1
126	Layered SiC sheets: A promising metal-free catalyst for NO reduction. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 60, 132-141.	2.4	17

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127	Reclamation of acid pickling waste: A facile route for preparation of single-phase Fe ₃ O ₄ nanoparticle. Journal of Magnetism and Magnetic Materials, 2015, 381, 401-404.	2.3	17
128	High stability and reactivity of defective graphene-supported Fe _n Pt _{13-n} (n=1, 2, and 3) nanoparticles for oxygen reduction reaction: a theoretical study. Journal of Nanoparticle Research, 2015, 17, 1.	1.9	9
129	Iron-chloride ionic liquid immobilized on SBA-15 for solvent-free oxidation of benzyl alcohol to benzaldehyde with H ₂ O ₂ . Chemical Engineering Science, 2015, 137, 268-275.	3.8	53
130	Iron-embedded boron nitride nanosheet as a promising electrocatalyst for the oxygen reduction reaction (ORR): A density functional theory (DFT) study. Journal of Power Sources, 2015, 287, 431-438.	7.8	99
131	High stability and superior catalytic reactivity of nitrogen-doped graphene supporting Pt nanoparticles as a catalyst for the oxygen reduction reaction: a density functional theory study. RSC Advances, 2015, 5, 34070-34077.	3.6	42
132	Fe ²⁺ and Co ²⁺ -embedded graphenes as electrocatalysts for the oxygen reduction reaction: theoretical insights. Physical Chemistry Chemical Physics, 2015, 17, 30687-30694.	2.8	48
133	Carbon-Doped Boron Nitride Nanosheet: An Efficient Metal-Free Electrocatalyst for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2015, 119, 26348-26354.	3.1	144
134	Hydroxyl-functionalized ionic liquid for activation and conversion of CO ₂ and methanol into dimethyl carbonate. Journal of CO ₂ Utilization, 2015, 12, 49-53.	6.8	25
135	Reclamation of Acid Pickling Waste: Preparation of Nano Fe ₂ O ₃ and Its Catalytic Performance. Industrial & Engineering Chemistry Research, 2014, 53, 20085-20091.	3.7	8
136	Theoretical Study on the Encapsulation of Li Atoms inside Boron Nitride Nanotubes: Physical Properties and Catalytic Reactivity for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2014, 118, 30325-30332.	3.1	11
137	Boosting sensitivity of boron nitride nanotube (BNNT) to nitrogen dioxide by Fe encapsulation. Journal of Molecular Graphics and Modelling, 2014, 51, 1-6.	2.4	23
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