Jing-xiang Zhao

List of Publications by Year
in descending order

179 papers	9,450 citations	44069 48 h-index	45317 90 g-index
179 all docs	179 docs citations	179 times ranked	8965 citing authors

#	Article	IF	Citations
1	Single Mo Atom Supported on Defective Boron Nitride Monolayer as an Efficient Electrocatalyst for Nitrogen Fixation: A Computational Study. Journal of the American Chemical Society, 2017, 139, 12480-12487.	13.7	1,006
2	Metal–Organic-Framework-Derived Fe-N/C Electrocatalyst with Five-Coordinated Fe-N$_x$ Sites for Advanced Oxygen Reduction in Acid Media. ACS Catalysis, 2017, 7, 1655-1663.	11.2	483
3	Computational Screening of Efficient Single‐Atom Catalysts Based on Graphitic Carbon Nitride (g‐C_3N_4) for Nitrogen Electroreduction. Small Methods, 2019, 3, 1800368.	8.6	347
4	Rational Design of Fe–N/C Hybrid for Enhanced Nitrogen Reduction Electrocatalysis under Ambient Conditions in Aqueous Solution. ACS Catalysis, 2019, 9, 336-344.	11.2	278
5	Coordination Number Regulation of Molybdenum Single-Atom Nanozyme Peroxidase-like Specificity. CheM, 2021, 7, 436-449.	11.7	216
6	Copper Dimer Supported on a C_2N 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
7	Single transition metal atom embedded into a MoS_2 nanosheet as a promising catalyst for electrochemical ammonia synthesis. Physical Chemistry Chemical Physics, 2018, 20, 9248-9255.	2.8	165
8	A boron-interstitial doped C_2N layer as a metal-free electrocatalyst for N_2 fixation: a computational study. Journal of Materials Chemistry A, 2019, 7, 2392-2399.	10.3	162
9	Phosphorene as a promising anchoring material for lithium–sulfur batteries: a computational study. Journal of Materials Chemistry A, 2016, 4, 6124-6130.	10.3	156
10	Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping. Small Methods, 2019, 3, 1800550.	8.6	149
11	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
12	Component Matters: Paving the Roadmap toward Enhanced Electrocatalytic Performance of Graphitic C_3N_4-Based Catalysts *via* Atomic Tuning. ACS Nano, 2017, 11, 6004-6014.	14.6	144
13	Computational screening of a single transition metal atom supported on the C_2N monolayer for electrochemical ammonia synthesis. Physical Chemistry Chemical Physics, 2018, 20, 12835-12844.	2.8	142
14	Coordination tunes the activity and selectivity of the nitrogen reduction reaction on single-atom iron catalysts: a computational study. Journal of Materials Chemistry A, 2021, 9, 1240-1251.	10.3	135
15	Phosphorus-doped graphene and (8, 0) carbon nanotube: Structural, electronic, magnetic properties, and chemical reactivity. Applied Surface Science, 2013, 273, 302-309.	6.1	133
16	Gas adsorption on silicene: A theoretical study. Computational Materials Science, 2014, 87, 218-226.	3.0	132
17	Polyoxometalate-based metal–organic framework-derived bimetallic hybrid materials for upgraded electrochemical reduction of nitrogen. Green Chemistry, 2020, 22, 6157-6169.	9.0	132
18	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

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19	Nitrogen electroreduction performance of transition metal dimers embedded into N-doped graphene: a theoretical prediction. Journal of Materials Chemistry A, 2020, 8, 4533-4543.	10.3	124
20	Construction of Z-scheme MoSe2/CdSe hollow nanostructure with enhanced full spectrum photocatalytic activity. Applied Catalysis B: Environmental, 2019, 244, 76-86.	20.2	122
21	Optimal Configuration of N‐Doped Carbon Defects in 2D Turbostratic Carbon Nanomesh for Advanced Oxygen Reduction Electrocatalysis. Angewandte Chemie - International Edition, 2020, 59, 11999-12006.	13.8	121
22	Construct of MoSe2/Bi2Se3 nanoheterostructure: Multimodal CT/PT imaging-guided PTT/PDT/chemotherapy for cancer treating. Biomaterials, 2019, 217, 119282.	11.4	119
23	Si-doped graphene: an ideal sensor for NO- or NO2-detection and metal-free catalyst for N2O-reduction. Journal of Molecular Modeling, 2012, 18, 2043-2054.	1.8	117
24	CO_2 electroreduction performance of a single transition metal atom supported on porphyrin-like graphene: a computational study. Physical Chemistry Chemical Physics, 2017, 19, 23113-23121.	2.8	117
25	Pyrrolic-nitrogen doped graphene: a metal-free electrocatalyst with high efficiency and selectivity for the reduction of carbon dioxide to formic acid: a computational study. Physical Chemistry Chemical Physics, 2016, 18, 5491-5498.	2.8	114
26	Revealing the Intrinsic Peroxidase-Like Catalytic Mechanism of Heterogeneous Single-Atom Co‐MoS2. Nano-Micro Letters, 2019, 11, 102.	27.0	114
27	Toward enhanced activity of a graphitic carbon nitride-based electrocatalyst in oxygen reduction and hydrogen evolution reactions via atomic sulfur doping. Journal of Materials Chemistry A, 2016, 4, 12205-12211.	10.3	112
28	Small Dopants Make Big Differences: Enhanced Electrocatalytic Performance of MoS2 Monolayer for Oxygen Reduction Reaction (ORR) by N‐ and P‐Doping. Electrochimica Acta, 2017, 225, 543-550.	5.2	106
29	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
30	A Co‐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
31	Silicon-Doped Graphene: An Effective and Metal-Free Catalyst for NO Reduction to N_2O?. ACS Applied Materials & Interfaces, 2013, 5, 5994-6000.	8.0	97
32	Removal of methylene blue from coloured effluents by adsorption onto SBA‐15. Journal of Chemical Technology and Biotechnology, 2011, 86, 616-619.	3.2	96
33	Elucidating the mechanism of the structure-dependent enzymatic activity of Fe‐N/C oxidase mimics. Chemical Communications, 2019, 55, 5271-5274.	4.1	95
34	Can Silicon Carbide Nanotubes Sense Carbon Dioxide?. Journal of Chemical Theory and Computation, 2009, 5, 1099-1105.	5.3	94
35	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_2H_4. Journal of Materials Chemistry A, 2019, 7, 4026-4035.	10.3	87
36	B-terminated (111) polar surfaces of BP and BAs: promising metal-free electrocatalysts with large reaction regions for nitrogen fixation. Journal of Materials Chemistry A, 2019, 7, 13284-13292.	10.3	87

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37	Intramolecular heterostructured carbon nitride with heptazine-triazine for enhanced photocatalytic hydrogen evolution. Chemical Engineering Journal, 2022, 428, 132579.	12.7	86
38	Si-embedded graphene: an efficient and metal-free catalyst for CO oxidation by N2O or O2. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	85
39	Highly selective oxidation of benzyl alcohol to benzaldehyde with hydrogen peroxide by biphasic catalysis. Chemical Engineering Journal, 2010, 162, 738-742.	12.7	82
40	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
41	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
42	Graphdiyne-Supported Single Iron Atom: A Promising Electrocatalyst for Carbon Dioxide Electroreduction into Methane and Ethanol. Journal of Physical Chemistry C, 2020, 124, 3722-3730.	3.1	75
43	Theoretical study on Si-doped hexagonal boron nitride (h -BN) sheet: Electronic, magnetic properties, and reactivity. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2989-2994.	2.1	74
44	Wet-chemistry hydrogen doped TiO2 with switchable defects control for photocatalytic hydrogen evolution. Matter, 2022, 5, 206-218.	10.0	66
45	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
46	Chemical functionalization of pyridine-like and porphyrin-like nitrogen-doped carbon (CN x) nanotubes with transition metal (TM) atoms: a theoretical study. Theoretical Chemistry Accounts, 2010, 127, 727-733.	1.4	53
47	Iron-chloride ionic liquid immobilized on SBA-15 for solvent-free oxidation of benzyl alcohol to benzaldehyde with H2O2. Chemical Engineering Science, 2015, 137, 268-275.	3.8	53
48	Single‑sided fluorine‑functionalized graphene: A metal‑free electrocatalyst with high efficiency for oxygen reduction reaction. Carbon, 2016, 104, 56-63.	10.3	51
49	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
50	Fe‑ and Co‑P_4-embedded graphenes as electrocatalysts for the oxygen reduction reaction: theoretical insights. Physical Chemistry Chemical Physics, 2015, 17, 30687-30694.	2.8	48
51	Stable Bimetallene Hydride Boosts Anodic CO Tolerance of Fuel Cells. ACS Energy Letters, 2021, 6, 1912-1919.	17.4	48
52	Solvent-free oxidation of toluene in an ionic liquid with H2O2 as oxidant. Chemical Engineering Journal, 2013, 225, 266-270.	12.7	45
53	Theoretical Study of the Deposition of Pt Clusters on Defective Hexagonal Boron Nitride (*h*-BN) Sheets: Morphologies, Electronic Structures, and Interactions with O. Journal of Physical Chemistry C, 2014, 118, 8868-8876.	3.1	45
54	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

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55	Electrochemical reduction of carbon dioxide on the two–dimensional M3(Hexaiminotriphenylene)2 sheet: A computational study. Applied Surface Science, 2019, 467-468, 98-103.	6.1	45
56	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
57	Two-dimensional π-conjugated metal bis(dithiolene) nanosheets as promising electrocatalysts for carbon dioxide reduction: a computational study. Journal of Materials Chemistry A, 2019, 7, 15341-15346.	10.3	40
58	Theoretical Prediction of the N–H and O–H Bonds Cleavage Catalyzed by the Single-Walled Silicon Carbide Nanotube. Journal of Physical Chemistry C, 2009, 113, 16736-16740.	3.1	39
59	Two-dimensional π-conjugated osmium bis(dithiolene) complex (OsC4S4) as a promising electrocatalyst for ambient nitrogen reduction to ammonia. Applied Surface Science, 2019, 487, 833-839.	6.1	39
60	A functionalized basic ionic liquid for synthesis of dimethyl carbonate from methanol and CO_2. Fuel Processing Technology, 2013, 115, 233-237.	7.2	38
61	Frustrated Lewis pairs photocatalyst for visible light-driven reduction of CO to multi-carbon chemicals. Nanoscale, 2019, 11, 20777-20784.	5.6	38
62	Theoretical Studies of the Interaction of an Open-Ended Boron Nitride Nanotube (BNNT) with Gas Molecules. Journal of Physical Chemistry C, 2008, 112, 20206-20211.	3.1	37
63	Divacancy-assisted transition metal adsorption on the BN graphene and its interaction with hydrogen molecules: a theoretical study. Applied Surface Science, 2013, 273, 293-301.	6.1	36
64	$FeMoO_4$ nanorods for efficient ambient electrochemical nitrogen reduction. Chemical Communications, 2020, 56, 6834-6837.	4.1	36
65	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
66	Selective synthesis of dimethyl carbonate from urea and methanol over Fe_2O_3/HMCM-49. Catalysis Science and Technology, 2012, 2, 305-309.	4.1	34
67	Stability and properties of the two-dimensional hexagonal boron nitride monolayer functionalized by hydroxyl (OH) radicals: a theoretical study. Journal of Molecular Modeling, 2013, 19, 5143-5152.	1.8	34
68	N-heterocyclic carbene as a promising metal-free electrocatalyst with high efficiency for nitrogen reduction to ammonia. Journal of Energy Chemistry, 2020, 46, 78-86.	12.9	33
69	SiC2 siligraphene as a promising anchoring material for lithium-sulfur batteries: a computational study. Applied Surface Science, 2018, 440, 889-896.	6.1	32
70	A Cu_2B_2 monolayer with planar hypercoordinate motifs: an efficient catalyst for CO electroreduction to ethanol. Journal of Materials Chemistry A, 2020, 8, 9607-9615.	10.3	32
71	Strain effect on the catalytic activities of B- and B/N-doped black phosphorene for electrochemical conversion of CO to valuable chemicals. Journal of Materials Chemistry A, 2020, 8, 11986-11995.	10.3	31
72	Revisiting catalytic performance of supported metal dimers for oxygen reduction reaction via magnetic coupling from first principles. , 2022, 1, 100031.		31

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73	Electrochemical conversion of CO2 into dimethyl carbonate in a functionalized ionic liquid. Journal of CO2 Utilization, 2013, 3-4, 98-101.	6.8	30
74	Computational screening of single-atom catalysts supported by VS_2 monolayers for electrocatalytic oxygen reduction/evolution reactions. Nanoscale, 2022, 14, 6902-6911.	5.6	30
75	Metal-N4/graphene as an efficient anchoring material for lithium-sulfur batteries: A computational study. Diamond and Related Materials, 2018, 90, 72-78.	3.9	29
76	Enhanced catalytic activity of MXene for nitrogen electoreduction reaction by carbon doping. Journal of Colloid and Interface Science, 2021, 588, 1-8.	9.4	29
77	Selective solvent-free oxidation of toluene to benzaldehyde over zeolite supported iron. Catalysis Communications, 2013, 39, 115-118.	3.3	28
78	Design and synthesis of surface-controlled CuOx/rGO nanocomposites with unusually high efficiency in catalytic conversion of organic reactants in the presence of NaBH4. Applied Surface Science, 2018, 459, 716-722.	6.1	28
79	CO oxidation catalyzed by silicon carbide (SiC) monolayer: A theoretical study. Journal of Molecular Graphics and Modelling, 2016, 66, 196-200.	2.4	27
80	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
81	Two-dimensional IrN2 monolayer: An efficient bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions. Journal of Colloid and Interface Science, 2021, 600, 711-718.	9.4	27
82	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
83	MoS2 â€" induced hollow Cu2O spheres: Synthesis and efficient catalytic performance in the reduction of 4-nitrophenol by NaBH4. Applied Surface Science, 2021, 539, 148285.	6.1	26
84	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
85	Electrochemical Conversion of Methanol and Carbon Dioxide to Dimethyl Carbonate at Graphite-Pt Electrode System. Journal of the Electrochemical Society, 2012, 159, E183-E186.	2.9	25
86	Hydroxyl-functionalized ionic liquid for activation and conversion of CO2 and methanol into dimethyl carbonate. Journal of CO2 Utilization, 2015, 12, 49-53.	6.8	25
87	Theoretical insights into the energetics and electronic properties of MPt12 (M = Fe, Co, Ni, Cu, and Pd) nanoparticles supported by N-doped defective graphene. Applied Surface Science, 2017, 397, 199-205.	6.1	25
88	Boosting ppb-level triethylamine sensing of ZnO: adjusting proportions of electron donor defects. Journal of Materials Chemistry C, 2020, 8, 6734-6742.	5.5	25
89	The effects of O_2 and H_2O adsorbates on field-emission properties of an (8, 0) boron nitride nanotube: a density functional theory study. Nanotechnology, 2009, 20, 085704.	2.6	24
90	Theoretical study on the encapsulation of Pd3-based transition metal clusters inside boron nitride nanotubes. Journal of Molecular Modeling, 2013, 19, 1143-1151.	1.8	23

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91	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
92	Modifying the electronic and magnetic properties of the boron nitride (BN) nanosheet by NHx (x=0, 1,) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.9	23
93	Theoretical investigation of the divacancies in boron nitride nanotubes: Properties and surface reactivity toward various adsorbates. Journal of Chemical Physics, 2009, 131, 014706.	3.0	22
94	Two-dimensional iron–tetracyanoquinodimethane (Fe–TCNQ) monolayer: an efficient electrocatalyst for the oxygen reduction reaction. RSC Advances, 2016, 6, 72952-72958.	3.6	22
95	RuN$_2$ Monolayer: A Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 54517-54523.	8.0	22
96	Flexible Pt$_3$Ni–S-Deposited Teflon Membrane with High Surface Mechanical Properties for Efficient Solar-Driven Strong Acidic/Alkaline Water Evaporation. ACS Applied Materials & Interfaces, 2020, 12, 27140-27149.	8.0	22
97	Chemical functionalization of BN graphene with the metal-arene group: a theoretical study. Journal of Materials Chemistry, 2012, 22, 9343.	6.7	21
98	Adsorption and catalytic activation of N2 molecule on iron dimer supported by different two-dimensional carbon-based substrates: A computational study. Applied Surface Science, 2020, 506, 144943.	6.1	21
99	Optimal Configuration of N–Doped Carbon Defects in 2D Turbostratic Carbon Nanomesh for Advanced Oxygen Reduction Electrocatalysis. Angewandte Chemie, 2020, 132, 12097-12104.	2.0	21
100	Theoretical study of the adsorption of CHO radicals on hexagonal boron nitride sheet: Structural and electronic changes. Applied Surface Science, 2014, 295, 137-143.	6.1	20
101	Experimental and theoretical investigation of the enhancement of the photo-oxidation of Hg0 by CeO2-modified morphology-controlled anatase TiO2. Journal of Hazardous Materials, 2021, 406, 124535.	12.4	20
102	Phthalocyanine-supported single-atom catalysts as a promising bifunctional electrocatalyst for ORR/OER: A computational study. ChemPhysMater, 2022, 1, 237-245.	2.8	20
103	Electrochemical synthesis of dimethyl carbonate from methanol, CO_2 and propylene oxide in an ionic liquid. Journal of Chemical Technology and Biotechnology, 2011, 86, 1413-1417.	3.2	19
104	Catalyst-free achieving of controllable carbon doping of boron nitride nanosheets by CO molecules: a theoretical prediction. RSC Advances, 2013, 3, 4917.	3.6	19
105	B$_4$C$_3$ Monolayer with Impressive Electronic, Optical, and Mechanical Properties: A Potential Metal-Free Photocatalyst for CO_2 Reduction under Visible Light. Journal of Physical Chemistry C, 2019, 123, 25091-25101.	3.1	19
106	Highly selective oxidation of styrene to benzaldehyde over Fe3O4 using H2O2 aqueous solution as oxidant. Reaction Kinetics, Mechanisms and Catalysis, 2018, 125, 743-756.	1.7	18
107	Highly selective synthesis of propylene glycol ether from methanol and propylene oxide catalyzed by basic ionic liquid. Journal of Chemical Technology and Biotechnology, 2011, 86, 105-108.	3.2	17
108	Layered SiC sheets: A promising metal-free catalyst for NO reduction. Journal of Molecular Graphics and Modelling, 2015, 60, 132-141.	2.4	17

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109	Reclamation of acid pickling waste: A facile route for preparation of single-phase Fe3O4 nanoparticle. Journal of Magnetism and Magnetic Materials, 2015, 381, 401-404.	2.3	17
110	A novel strategy for conversion of methanol and CO2 into dimethoxymethane in a basic ionic liquid. Journal of Molecular Catalysis A, 2016, 421, 117-121.	4.8	17
111	Heterostructures of doped graphene and MoX$_2$ (X = S and Se) as promising anchoring materials for lithium–sulfur batteries: a first-principles study. New Journal of Chemistry, 2019, 43, 9396-9402.	2.8	17
112	VOx molecular level grafted g-C3N4 for highly selective oxidation of methanol to dimethoxymethane. Molecular Catalysis, 2019, 469, 48-56.	2.0	17
113	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
114	Supported Cu$_3$ clusters on graphitic carbon nitride as an efficient catalyst for CO electroreduction to propene. Journal of Materials Chemistry A, 2022, 10, 14460-14469.	10.3	17
115	A DFT/B3LYP Computational Study of Boron–Nitride Nanotubes. Journal of the Chinese Chemical Society, 2003, 50, 525-528.	1.4	16
116	Chemical functionalization of graphene via aryne cycloaddition: a theoretical study. Journal of Molecular Modeling, 2012, 18, 2861-2868.	1.8	16
117	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
118	An organic polymer-grafted ionic liquid as a catalyst for the cycloaddition of CO$_2$ to epoxides. New Journal of Chemistry, 2017, 41, 387-392.	2.8	15
119	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
120	Single Mn atom as a promising electrocatalyst for CO reduction to C2H5OH and C3H6: A computational study. Applied Surface Science, 2019, 498, 143868.	6.1	15
121	Two-dimensional π-conjugated metal bis(dithiolene) nanosheet: A promising anchoring material for lithium-sulfur batteries. Computational Materials Science, 2020, 171, 109228.	3.0	15
122	Fe3 Cluster Anchored on the C2N Monolayer for Efficient Electrochemical Nitrogen Fixation. Catalysts, 2020, 10, 974.	3.5	15
123	Size-dependent electrocatalytic activity of ORR/OER on palladium nanoclusters anchored on defective MoS$_2$ monolayers. New Journal of Chemistry, 2020, 44, 16135-16143.	2.8	15
124	2D Bismuthene Metal Electron Mediator Engineering Super Interfacial Charge Transfer for Efficient Photocatalytic Reduction of Carbon Dioxide. ACS Applied Materials & Interfaces, 2021, 13, 21582-21592.	8.0	15
125	P- or S-Doped graphdiyne as a superior metal-free electrocatalyst for the hydrogen evolution reaction: a computational study. New Journal of Chemistry, 2021, 45, 8101-8108.	2.8	14
126	Synthesis of a Co–Sn Alloy-Deposited PTFE Film for Enhanced Solar-Driven Water Evaporation via a Super-Absorbent Polymer-Based "Water Pump" Design. ACS Applied Materials & Interfaces, 2021, 13, 26879-26890.	8.0	14

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127	A density functional theory study of the adsorption of bimetallic Fe n Pt m clusters on defective graphene: structural, electronic, and magnetic properties. Journal of Nanoparticle Research, 2013, 15, 1.	1.9	13
128	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
129	Controlled 2H/1T phase transition in MoS_2 monolayers by a strong interface with M_2C MXenes: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 20107-20116.	2.8	13
130	A metallic Cu_2N monolayer with planar tetracoordinated nitrogen as a promising catalyst for CO_2 electroreduction. Journal of Materials Chemistry A, 2022, 10, 1560-1568.	10.3	13
131	Theoretical study of oxidation of monovacancies in hexagonal boron nitride (h-BN) sheet by oxygen molecules. Journal of Molecular Modeling, 2014, 20, 2197.	1.8	12
132	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
133	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
134	Transformation of ZIF-8 nanoparticles into 3D nitrogen-doped hierarchically porous carbon for Li–S batteries. RSC Advances, 2020, 10, 17345-17352.	3.6	12
135	Single transition metal atoms anchored on a C_2N monolayer as efficient catalysts for hydrazine electrooxidation. Physical Chemistry Chemical Physics, 2020, 22, 16691-16700.	2.8	12
136	A Simple Polyoxometallate for Selective Oxidation of Benzyl Alcohol to Benzaldehyde with Hydrogen Peroxide. Chinese Journal of Chemistry, 2012, 30, 433-437.	4.9	11
137	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
138	Pyridine derivative/graphene nanoribbon composites as molecularly tunable heterogeneous electrocatalysts for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2016, 18, 5040-5047.	2.8	11
139	Highly selective oxidation of methanol to dimethoxymethane over SO_4^{2-}/V_2O_5–ZrO_2. New Journal of Chemistry, 2017, 41, 8370-8376.	2.8	11
140	PtN_3-Embedded graphene as an efficient catalyst for electrochemical reduction of nitrobenzene to aniline: a theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 17639-17645.	2.8	11
141	Tuneable oxidation of styrene to benzaldehyde and benzoic acid over Co/ZSM-5. New Journal of Chemistry, 2021, 45, 18192-18201.	2.8	11
142	Mo–Vacancies Defect Engineering of One–Dimensional Porous Mo_2C Nanowires for Enhanced High–Efficiency Hydrogen Evolution. ChemCatChem, 0, , .	3.7	11
143	Theoretical study of phenol adsorption on the (8, 0) silicon carbide nanotube. Theoretical Chemistry Accounts, 2011, 129, 85-92.	1.4	10
144	Theoretical insights into the effects of the diameter and helicity on the adsorption of formic acid on silicon carbide nanotube. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	10

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145	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
146	Highly Selective Oxidation of Styrene Over FeCl3-Imidazolium Ionic Liquid Grafted SBA-15. Catalysis Letters, 2019, 149, 2994-2999.	2.6	10
147	Tuning the electronic structures of monolayer triphosphides MP_3 (M = Sn and Ge) for CO_2 electroreduction through interface engineering: a theoretical prediction. Physical Chemistry Chemical Physics, 2020, 22, 6896-6905.	2.8	10
148	An atom-economic reaction for synthesis of 1-phenoxy-2-propanol over Al2O3/MgO. Applied Catalysis A: General, 2011, 408, 125-129.	4.3	9
149	High stability and reactivity of defective graphene-supported Fe n Pt13−n (n=1, 2, and 3) nanoparticles for oxygen reduction reaction: a theoretical study. Journal of Nanoparticle Research, 2015, 17, 1.	1.9	9
150	Doping MoS2 monolayer with nonmetal atoms to tune its electronic and magnetic properties, and chemical activity: a computational study. New Journal of Chemistry, 2019, 43, 5766-5772.	2.8	9
151	Photodegradation of naphthalene over Fe 3 O 4 under visible light irradiation. Royal Society Open Science, 2019, 6, 181779.	2.4	9
152	Copper vanadate nanowires on g-C3N4 toward highly selective oxidation of methanol to dimethoxymethane. Applied Surface Science, 2021, 548, 149180.	6.1	9
153	Capture and catalytic conversion of lithium polysulfides by metal-doped MoS2 monolayers for lithium–sulfur batteries: A computational study. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 130, 114715.	2.7	9
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155	Theoretical prediction of the mechanisms for defect healing or oxygen doping in a hexagonal boron nitride (h-BN) sheet with nitrogen vacancies by NO2 molecules. Journal of Molecular Modeling, 2014, 20, 2307.	1.8	8
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