

# Zi-Qi Tian

## List of Publications by Citations

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116  
papers

4,406  
citations

34  
h-index

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g-index

123  
ext. papers

5,834  
ext. citations

9.1  
avg, IF

6.11  
L-index

#	Paper	IF	Citations
116	Electrochemical Ammonia Synthesis via Nitrogen Reduction Reaction on a MoS Catalyst: Theoretical and Experimental Studies. <i>Advanced Materials</i> , <b>2018</b> , 30, e1800191	24	524
115	Electrochemical N fixation to NH under ambient conditions: MoN nanorod as a highly efficient and selective catalyst. <i>Chemical Communications</i> , <b>2018</b> , 54, 8474-8477	5.8	224
114	High-Performance Electrohydrogenation of N <sub>2</sub> to NH <sub>3</sub> Catalyzed by Multishelled Hollow Cr <sub>2</sub> O <sub>3</sub> Microspheres under Ambient Conditions. <i>ACS Catalysis</i> , <b>2018</b> , 8, 8540-8544	13.1	218
113	Multi-Molar Absorption of CO <sub>2</sub> by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 7166-70	16.4	212
112	Chromium-ruthenium oxide solid solution electrocatalyst for highly efficient oxygen evolution reaction in acidic media. <i>Nature Communications</i> , <b>2019</b> , 10, 162	17.4	201
111	Assembling Ultrasmall Copper-Doped Ruthenium Oxide Nanocrystals into Hollow Porous Polyhedra: Highly Robust Electrocatalysts for Oxygen Evolution in Acidic Media. <i>Advanced Materials</i> , <b>2018</b> , 30, e1801351	24	199
110	Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction. <i>Small Methods</i> , <b>2019</b> , 3, 1900337	12.8	124
109	Regulating the Electronic Structure of CoP Nanosheets by O Incorporation for High-Efficiency Electrochemical Overall Water Splitting. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 1905252	15.6	124
108	Fabricating Single-Atom Catalysts from Chelating Metal in Open Frameworks. <i>Advanced Materials</i> , <b>2019</b> , 31, e1808193	24	103
107	Ultrafine Defective RuO <sub>2</sub> Electrocatalyst Integrated on Carbon Cloth for Robust Water Oxidation in Acidic Media. <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1901313	21.8	95
106	Hexagonal boron nitride nanosheet for effective ambient N <sub>2</sub> fixation to NH <sub>3</sub> . <i>Nano Research</i> , <b>2019</b> , 12, 919-924	10	88
105	Ion-Gated Gas Separation through Porous Graphene. <i>Nano Letters</i> , <b>2017</b> , 17, 1802-1807	11.5	84
104	Selective Charging Behavior in an Ionic Mixture Electrolyte-Supercapacitor System for Higher Energy and Power. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 18681-18687	16.4	76
103	In Situ Anchoring Polymetallic Phosphide Nanoparticles within Porous Prussian Blue Analogue Nanocages for Boosting Oxygen Evolution Catalysis. <i>Nano Letters</i> , <b>2021</b> , 21, 3016-3025	11.5	75
102	Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 6843-6847	16.4	63
101	Interactions between Antibiotics and Graphene-Based Materials in Water: A Comparative Experimental and Theoretical Investigation. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 24273-80	9.5	61
100	Ammonia Thermal Treatment toward Topological Defects in Porous Carbon for Enhanced Carbon Dioxide Electroreduction. <i>Advanced Materials</i> , <b>2020</b> , 32, e2001300	24	60

99	Insight into adsorption of combined antibiotic-heavy metal contaminants on graphene oxide in water. <i>Separation and Purification Technology</i> , <b>2020</b> , 236, 116278	8.3	58
98	Expanded Porphyrins as Two-Dimensional Porous Membranes for CO <sub>2</sub> Separation. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 13073-9	9.5	55
97	The ligand effect on the isomer stability of Au <sub>24</sub> (SR) <sub>20</sub> clusters. <i>Nanoscale</i> , <b>2015</b> , 7, 2225-9	7.7	50
96	C-O versus C-C bond cleavage: selectivity control in Lewis acid catalyzed chemodivergent cycloadditions of aryl oxiranyldicarboxylates with aldehydes, and theoretical rationalizations of reaction pathways. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 8591-5	4.8	50
95	Theoretical Investigation on the Single Transition-Metal Atom-Decorated Defective MoS <sub>2</sub> for Electrocatalytic Ammonia Synthesis. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 36506-36514	9.5	49
94	The N-B Interaction through a Water Bridge: Understanding the Chemoselectivity of a Fluorescent Protein Based Probe for Peroxynitrite. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 4900-7	16.4	49
93	Scale inhibition performance and mechanism of sulfamic/amino acids modified polyaspartic acid against calcium sulfate. <i>Desalination</i> , <b>2017</b> , 419, 152-159	10.3	48
92	Rational design and synthesis of a porous, task-specific polycarbazole for efficient CO <sub>2</sub> capture. <i>Chemical Communications</i> , <b>2016</b> , 52, 4454-7	5.8	47
91	Highly efficient N fixation catalysts: transition-metal carbides MC (MXenes). <i>Nanoscale</i> , <b>2020</b> , 12, 538-547	7.7	46
90	Removal of antibiotics from water in the coexistence of suspended particles and natural organic matters using amino-acid-modified-chitosan flocculants: A combined experimental and theoretical study. <i>Journal of Hazardous Materials</i> , <b>2016</b> , 317, 593-601	12.8	46
89	Separation and Sequential Recovery of Tetracycline and Cu(II) from Water Using Reusable Thermoresponsive Chitosan-Based Flocculant. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 10266-10275	9.5	42
88	Phenothiazine-anthraquinone donor-acceptor molecules: synthesis, electronic properties and DFT-TDDFT computational study. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 9997-10004	2.8	39
87	Identify the Removable Substructure in Carbon Activation. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 7288-7295	9.6	38
86	Atomically dispersed Lewis acid sites boost 2-electron oxygen reduction activity of carbon-based catalysts. <i>Nature Communications</i> , <b>2020</b> , 11, 5478	17.4	38
85	Recent Progress in the Theoretical Investigation of Electrocatalytic Reduction of CO <sub>2</sub> . <i>Advanced Theory and Simulations</i> , <b>2018</b> , 1, 1800004	3.5	37
84	Enhanced removal of trace antibiotics from turbid water in the coexistence of natural organic matters using phenylalanine-modified-chitosan flocculants: Effect of flocculants' molecular architectures. <i>Chemical Engineering Journal</i> , <b>2018</b> , 333, 310-319	14.7	37
83	Multi-Molar Absorption of CO <sub>2</sub> by the Activation of Carboxylate Groups in Amino Acid Ionic Liquids. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 7282-7286	3.6	35
82	Flocculation of different types of combined contaminants of antibiotics and heavy metals by thermo-responsive flocculants with various architectures. <i>Separation and Purification Technology</i> , <b>2019</b> , 223, 123-132	8.3	34

81	Light- and Electric-Field-Induced Switching of Thiolated Azobenzene Self-Assembled Monolayer. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 19934-19944	3.8	33
80	Substitution Effect Guided Synthesis of Task-Specific Nanoporous Polycarbazoles with Enhanced Carbon Capture. <i>Macromolecules</i> , <b>2016</b> , 49, 5325-5330	5.5	32
79	Anion-Functionalized Task-Specific Ionic Liquids: Molecular Origin of Change in Viscosity upon CO <sub>2</sub> Capture. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 14880-7	3.4	32
78	Reactive molecular dynamics simulations of switching processes of azobenzene-based monolayer on surface. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 014706	3.9	32
77	Size-selective adsorption of methyl orange using a novel nano-composite by encapsulating HKUST-1 in hyper-crosslinked polystyrene networks. <i>Journal of Cleaner Production</i> , <b>2018</b> , 184, 949-958	10.3	31
76	Intrinsic defects in biomass-derived carbons facilitate electroreduction of CO <sub>2</sub> . <i>Nano Research</i> , <b>2020</b> , 13, 729-735	10	30
75	Porous rod-like Ni <sub>2</sub> P/Ni assemblies for enhanced urea electrooxidation. <i>Nano Research</i> , <b>2021</b> , 14, 1405-1412	11.2	30
74	Enhanced adsorption of pharmaceuticals onto core-brush shaped aromatic rings-functionalized chitosan magnetic composite particles: Effects of structural characteristics of both pharmaceuticals and brushes. <i>Journal of Cleaner Production</i> , <b>2018</b> , 172, 1025-1034	10.3	30
73	Stability and Core-Level Signature of Nitrogen Dopants in Carbonaceous Materials. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 5775-5781	9.6	29
72	Role of moderately hydrophobic chitosan flocculants in the removal of trace antibiotics from water and membrane fouling control. <i>Water Research</i> , <b>2020</b> , 177, 115775	12.5	28
71	What can molecular simulation do for global warming?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2016</b> , 6, 173-197	7.9	28
70	Transitional Metal Catalytic Pyrite Cathode Enables Ultrastable Four-Electron-Based All-Solid-State Lithium Batteries. <i>ACS Nano</i> , <b>2019</b> , 13, 9551-9560	16.7	28
69	Ab Initio Screening of CO <sub>2</sub> -philic Groups. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3848-52	2.8	24
68	Effect of pore density on gas permeation through nanoporous graphene membranes. <i>Nanoscale</i> , <b>2018</b> , 10, 14660-14666	7.7	23
67	Efficient adsorptive desulfurization by task-specific porous organic polymers. <i>AIChE Journal</i> , <b>2016</b> , 62, 1740-1746	3.6	23
66	Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 6947-6951	3.6	22
65	Electronic modulation by N incorporation boosts the electrocatalytic performance of urchin-like Ni <sub>5</sub> P <sub>4</sub> hollow microspheres for hydrogen evolution. <i>Chemical Engineering Journal</i> , <b>2020</b> , 402, 126302	14.7	22
64	Impact of tuning CO <sub>2</sub> -philicity in polydimethylsiloxane-based membranes for carbon dioxide separation. <i>Journal of Membrane Science</i> , <b>2017</b> , 530, 213-219	9.6	21

63	Enhanced visible light photocatalytic activity for the hybrid MoS <sub>2</sub> /anatase TiO <sub>2</sub> (0 0 1) nanocomposite: A first-principles study. <i>Chemical Physics Letters</i> , <b>2014</b> , 612, 285-288	2.5	21
62	First-principles molecular dynamics simulation of the Ca <sub>2</sub> UO <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> complex in water. <i>Dalton Transactions</i> , <b>2016</b> , 45, 9812-9	4.3	20
61	Norfloxacin and Bisphenol-A Removal Using Temperature-Switchable Graphene Oxide. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 29083-29091	9.5	20
60	Supported bicyclic amidine ionic liquids as a potential CO <sub>2</sub> /N <sub>2</sub> separation medium. <i>Journal of Membrane Science</i> , <b>2018</b> , 565, 203-212	9.6	20
59	Enhanced selective adsorption of benzotriazole onto nanosized zeolitic imidazolate frameworks confined in polystyrene anion exchanger. <i>Chemical Engineering Journal</i> , <b>2017</b> , 328, 816-824	14.7	20
58	Heterogeneous single-cluster catalysts (Mn <sub>3</sub> , Fe <sub>3</sub> , Co <sub>3</sub> , and Mo <sub>3</sub> ) supported on nitrogen-doped graphene for robust electrochemical nitrogen reduction. <i>Journal of Energy Chemistry</i> , <b>2021</b> , 54, 612-619 <sup>12</sup>	19	19
57	Deep Eutectic Solvents Formed by N-Methylacetamide and Heterocyclic Weak Acids for Highly Efficient and Reversible Chemical Absorption of Ammonia. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2020</b> , 59, 2060-2067	3.9	18
56	Rhodium-Catalyzed Expedient Synthesis of Indenes from Propargyl Alcohols and Organoboronic Acids by Selective 1,4-Rhodium Migration over $\beta$ Oxygen Elimination. <i>ACS Catalysis</i> , <b>2019</b> , 9, 6857-6863	13.1	18
55	Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp <sup>2</sup> -c-COF. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 43595-43602	9.5	17
54	Tuning Ion-Pair Interaction in Cuprous-Based Protic Ionic Liquids for Significantly Improved CO Capture. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 11894-11900	8.3	16
53	Efficient adsorption of four phenolic compounds using a robust nanocomposite fabricated by confining 2D porous organic polymers in 3D anion exchangers. <i>Chemical Engineering Journal</i> , <b>2020</b> , 396, 125296	14.7	16
52	Site Partition: Turning One Site into Two for Adsorbing CO <sub>2</sub> . <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 2568-72	6.4	15
51	Theoretical design of visible light driven azobenzene-based photo-switching molecules. <i>Chemical Physics Letters</i> , <b>2014</b> , 613, 110-114	2.5	15
50	Bimetallic Metal-Organic Framework with High-Adsorption Capacity toward Lithium Polysulfides for Lithium-Sulfur Batteries. <i>Energy and Environmental Materials</i> ,	13	15
49	Monitoring graphene oxide's efficiency for removing Re(VII) and Cr(VI) with fluorescent silica hydrogels. <i>Environmental Pollution</i> , <b>2020</b> , 262, 114246	9.3	14
48	Synthesis, characterization and electrochemiluminescent properties of cyclometalated platinum(II) complexes with substituted 2-phenylpyridine ligands. <i>Dalton Transactions</i> , <b>2013</b> , 42, 4059-67	4.3	14
47	Dynamic simulations of stimuli-responsive switching of azobenzene derivatives in self-assembled monolayers: reactive rotation potential and switching functions. <i>Molecular Simulation</i> , <b>2015</b> , 41, 28-42	2	13
46	Chiral interconversions of Pd and/or Au bis-metalated [32]octaphyrins(1,0,1,0,1,0,1,0) involving Hückel and Möbius macrocyclic topologies: a theoretical prediction. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 8124-30	4.2	13

45	Synergistic effects of heteroatom-decorated MXene catalysts for CO reduction reactions. <i>Nanoscale</i> , <b>2020</b> , 12, 15880-15887	7.7	13
44	High-Throughput Screening of a Single-Atom Alloy for Electroreduction of Dinitrogen to Ammonia. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 16336-16344	9.5	13
43	Confined Ionic Liquid in an Ionic Porous Aromatic Framework for Gas Separation. <i>ACS Applied Polymer Materials</i> , <b>2019</b> , 1, 95-102	4.3	13
42	Environmental-friendly one-step fabrication of tertiary amine-functionalized adsorption resins for removal of benzophenone-4 from water. <i>Journal of Cleaner Production</i> , <b>2018</b> , 203, 655-663	10.3	13
41	Pd-Metalated Conjugated Nanoporous Polycarbazoles for Additive-Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. <i>ChemSusChem</i> , <b>2017</b> , 10, 2348-2351	8.3	12
40	Control of Chemoselectivity by Coordinated Water and Relative Size of Ligands to Metal Cations of Lewis Acid Catalysts for Cycloaddition of an Oxirane Derivative to an Aldehyde: Theoretical and Experimental Study. <i>Organometallics</i> , <b>2014</b> , 33, 1715-1725	3.8	12
39	Theoretical insight into azobis-(benzo-18-crown-6) ether combined with the alkaline earth metal cations. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1066, 28-33	2	12
38	Thermally regulated molybdate-based ionic liquids toward molecular oxygen activation for one-pot oxidative cascade catalysis. <i>Green Chemistry</i> , <b>2020</b> , 22, 103-109	10	11
37	Visible/infrared light-driven high-efficiency CO <sub>2</sub> conversion into ethane based on a BiO synergistic catalyst. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 22327-22334	13	11
36	Use of steric encumbrance to develop conjugated nanoporous polymers for metal-free catalytic hydrogenation. <i>Chemical Communications</i> , <b>2016</b> , 52, 11919-11922	5.8	11
35	The Critical Role of Additive Sulfate for Stable Alkaline Seawater Oxidation on Nickel-Based Electrodes. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 22740-22744	16.4	11
34	Theoretical Framework of 1,3-Thiazolium-5-Thiolates Mesoionic Compounds: Exploring the Nature of Photophysical Property and Molecular Nonlinearity. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 5563-5569	2.8	10
33	FeP/MoS <sub>2</sub> Enriched with Dense Catalytic Sites and High Electrical Conductivity for the Hydrogen Evolution Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 17671-17681	8.3	10
32	Tuning the collective switching behavior of azobenzene/Au hybrid materials: flexible versus rigid azobenzene backbones and Au(111) surfaces versus curved Au nanoparticles. <i>Nanoscale</i> , <b>2017</b> , 9, 16700-16710	7.7	10
31	Oxygen vacancies in Bi <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub> quantum dots to trigger efficient photocatalytic nitrogen reduction. <i>Applied Catalysis B: Environmental</i> , <b>2021</b> , 299, 120680	21.8	9
30	Atomically Dispersed Mo Sites Anchored on Multichannel Carbon Nanofibers toward Superior Electrocatalytic Hydrogen Evolution. <i>ACS Nano</i> , <b>2021</b> ,	16.7	8
29	Fast and Stable Electrochemical Production of H <sub>2</sub> O <sub>2</sub> by Electrode Architecture Engineering. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2021</b> , 9, 7120-7129	8.3	8
28	Enhancement of Mass Transfer for Facilitating Industrial-Level CO <sub>2</sub> Electroreduction on Atomic Ni <sub>2</sub> N <sub>4</sub> Sites. <i>Advanced Energy Materials</i> , <b>2021</b> , 11, 2102152	21.8	8

27	Optimal Size of a Cylindrical Pore for Post-Combustion CO <sub>2</sub> Capture. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 22025-22030	3.8	7
26	Ionic liquid-induced graphitization of biochar: N/P dual-doped carbon nanosheets for high-performance lithium/sodium storage. <i>Journal of Materials Science</i> , <b>2021</b> , 56, 8186-8201	4.3	7
25	Eco-friendly utilization of sawdust: Ionic liquid-modified biochar for enhanced Li storage of TiO <sub>2</sub> . <i>Science of the Total Environment</i> , <b>2021</b> , 794, 148688	10.2	7
24	Design of Calix-Based Cages for CO <sub>2</sub> Capture. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2017</b> , 56, 4502-4507	3.9	6
23	Double Atom Catalysts: Heteronuclear Transition Metal Dimer Anchored on Nitrogen-Doped Graphene as Superior Electrocatalyst for Nitrogen Reduction Reaction. <i>Advanced Theory and Simulations</i> , <b>2020</b> , 3, 2000190	3.5	6
22	Ionic liquid-induced low temperature graphitization of cellulose-derived biochar for high performance sodium storage. <i>Surface and Coatings Technology</i> , <b>2021</b> , 412, 127034	4.4	6
21	Enhanced scale inhibition against Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> and Fe <sub>2</sub> O <sub>3</sub> in water using multi-functional fluorescently-tagged antibacterial scale inhibitors. <i>Environmental Science: Water Research and Technology</i> , <b>2020</b> , 6, 951-962	4.2	5
20	Ligand Defect Density Regulation in Metal-Organic Frameworks by Functional Group Engineering on Linkers.. <i>Nano Letters</i> , <b>2022</b> ,	11.5	5
19	Comparative Reaction Diagrams for the SN(2) Reaction Formulated According to the Leffler Analysis and the Hammond Postulate. <i>Journal of Organic Chemistry</i> , <b>2016</b> , 81, 3648-53	4.2	4
18	Hydrophobic-modified metal-hydroxide nanofloculants enable one-step removal of multi-contaminants for drinking water production. <i>IScience</i> , <b>2021</b> , 24, 102491	6.1	3
17	Confinement of sulfur-doped NiO nanoparticles into N-doped carbon nanotube/nanofiber-coupled hierarchical branched superstructures: Electronic modulation by anion doping boosts oxygen evolution electrocatalysis. <i>Journal of Energy Chemistry</i> , <b>2021</b> , 63, 585-585	12	3
16	Application of ultra-low concentrations of moderately-hydrophobic chitosan for ultrafiltration membrane fouling mitigation. <i>Journal of Membrane Science</i> , <b>2021</b> , 635, 119540	9.6	3
15	Electrocatalysts: Ultrafine Defective RuO <sub>2</sub> Electrocatalyst Integrated on Carbon Cloth for Robust Water Oxidation in Acidic Media (Adv. Energy Mater. 35/2019). <i>Advanced Energy Materials</i> , <b>2019</b> , 9, 1970136	21.8	2
14	Theoretical design and computational simulations of visible light driven azobenzene-based switches. <i>Scientia Sinica Chimica</i> , <b>2015</b> , 45, 412-418	1.6	2
13	Electron-donating groups and high ring strain promoted ring opening of methylenecyclopropanes catalyzed by rhodium and iridium complexes. <i>Journal of Organometallic Chemistry</i> , <b>2016</b> , 811, 29-39	2.3	2
12	The Critical Role of Additive Sulfate for Stable Alkaline Seawater Oxidation on Nickel-Based Electrodes. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 22922	3.6	2
11	Enhanced catalytic performance of Pt by coupling with carbon defects. <i>Innovation(China)</i> , <b>2021</b> , 2, 1001617.8	17.8	2
10	Theoretical investigation of defective MXenes as potential electrocatalysts for CO reduction toward C products. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 12431-12438	3.6	2

9	Theoretical Screening of Transition Metal Doped Defective MoS as Efficient Electrocatalyst for CO Conversion to CH. <i>ChemPhysChem</i> , <b>2021</b> ,	3.2	1
8	Theoretical Study on the Electrochemical Catalytic Activity of Au-Doped Pt Electrode for Nitrogen Monoxide. <i>Chemosensors</i> , <b>2022</b> , 10, 178	4	1
7	Influence of DOM characteristics on the flocculation removal of trace pharmaceuticals in surface water by the successive dosing of alum and moderately hydrophobic chitosan.. <i>Water Research</i> , <b>2022</b> , 213, 118163	12.5	0
6	Understanding the CO <sub>2</sub> /CH <sub>4</sub> /N <sub>2</sub> Separation Performance of Nanoporous Amorphous N-Doped Carbon Combined Hybrid Monte Carlo with Machine Learning. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 2100378 <sup>3.5</sup>		0
5	Investigation on a Zr-based metal-organic framework (MOF-801) for the high-performance separation of light alkanes. <i>Chemical Communications</i> , <b>2021</b> , 57, 13008-13011	5.8	0
4	Ultrathin Membranes for Gas Separation <b>2020</b> , 153-185		0
3	Reaping the catalytic benefits of both surface (NiFe <sub>2</sub> O <sub>4</sub> ) and underneath (Ni <sub>3</sub> Fe) layers for the oxygen evolution reaction. <i>Sustainable Energy and Fuels</i> , <b>2021</b> , 5, 2704-2714	5.8	0
2	Rücktitelbild: Highly Efficient Carbon Monoxide Capture by Carbanion-Functionalized Ionic Liquids through C-Site Interactions (Angew. Chem. 24/2017). <i>Angewandte Chemie</i> , <b>2017</b> , 129, 7108-7108	3.6	
1	Pd-Metalated Conjugated Nanoporous Polycarbazoles for Additive-Free Cyanation of Aryl Halides: Boosting Catalytic Efficiency through Spatial Modulation. <i>ChemSusChem</i> , <b>2017</b> , 10, 2320-2320	8.3	