

# Zi-Qi Tian

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

116  
papers

4,406  
citations

34  
h-index

63  
g-index

123  
ext. papers

5,834  
ext. citations

9.1  
avg. IF

6.11  
L-index

#	Paper	IF	Citations
116	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
115	Ligand Defect Density Regulation in Metal-Organic Frameworks by Functional Group Engineering on Linkers.. <i>Nano Letters</i> , <b>2022</b> ,	11.5	5
114	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
113	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
112	Atomically Dispersed Mo Sites Anchored on Multichannel Carbon Nanofibers toward Superior Electrocatalytic Hydrogen Evolution. <i>ACS Nano</i> , <b>2021</b> ,	16.7	8
111	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
110	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
109	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
108	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
107	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
106	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
105	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
104	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>	12	19
103	Porous rod-like Ni <sub>2</sub> P/Ni assemblies for enhanced urea electrooxidation. <i>Nano Research</i> , <b>2021</b> , 14, 1405-1412	14.1	30
102	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
101	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
100	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

99	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
98	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
97	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
96	Enhanced catalytic performance of Pt by coupling with carbon defects. <i>Innovation(China)</i> , <b>2021</b> , 2, 1001617.8	17.8	2
95	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
94	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
93	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
92	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
91	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
90	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
89	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
88	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
87	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
86	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
85	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
84	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
83	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
82	Highly efficient N fixation catalysts: transition-metal carbides MC (MXenes). <i>Nanoscale</i> , <b>2020</b> , 12, 538-547.7	7.7	46

81	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
80	Ultrathin Membranes for Gas Separation <b>2020</b> , 153-185		0
79	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
78	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
77	Synergistic effects of heteroatom-decorated MXene catalysts for CO reduction reactions. <i>Nanoscale</i> , <b>2020</b> , 12, 15880-15887	7.7	13
76	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
75	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
74	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
73	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
72	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
71	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
70	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
69	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
68	Fabricating Single-Atom Catalysts from Chelating Metal in Open Frameworks. <i>Advanced Materials</i> , <b>2019</b> , 31, e1808193	24	103
67	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
66	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
65	Rhodium-Catalyzed Expeditious 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
64	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

63	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
62	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
61	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
60	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
59	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
58	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
57	Effect of pore density on gas permeation through nanoporous graphene membranes. <i>Nanoscale</i> , <b>2018</b> , 10, 14660-14666	7.7	23
56	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
55	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
54	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
53	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
52	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
51	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
50	Electrochemical Ammonia Synthesis via Nitrogen Reduction Reaction on a MoS <sub>2</sub> Catalyst: Theoretical and Experimental Studies. <i>Advanced Materials</i> , <b>2018</b> , 30, e1800191	24	524
49	Electrochemical N fixation to NH <sub>3</sub> 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
48	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
47	Ion-Gated Gas Separation through Porous Graphene. <i>Nano Letters</i> , <b>2017</b> , 17, 1802-1807	11.5	84
46	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

45	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
44	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	
43	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
42	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	
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	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
39	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 <sup>9</sup>	7.7	10 <sup>9</sup>
38	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
37	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
36	Identify the Removable Substructure in Carbon Activation. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 7288-7295	9.6	38
35	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
34	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
33	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
32	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
31	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
30	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
29	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
28	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



27	First-principles molecular dynamics simulation of the $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3$ complex in water. <i>Dalton Transactions</i> , <b>2016</b> , 45, 9812-9	4.3	20
26	Multi-Molar Absorption of $\text{CO}_2$ 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
25	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
24	Efficient adsorptive desulfurization by task-specific porous organic polymers. <i>AIChE Journal</i> , <b>2016</b> , 62, 1740-1746	3.6	23
23	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
22	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
21	Comparative Reaction Diagrams for the $\text{S}_\text{N}(2)$ 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
20	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
19	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
18	Expanded Porphyrins as Two-Dimensional Porous Membranes for $\text{CO}_2$ Separation. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 13073-9	9.5	55
17	Ab Initio Screening of $\text{CO}_2$ -philic Groups. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3848-52	2.8	24
16	The ligand effect on the isomer stability of $\text{Au}_{24}(\text{SR})_{20}$ clusters. <i>Nanoscale</i> , <b>2015</b> , 7, 2225-9	7.7	50
15	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
14	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
13	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
12	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
11	Enhanced visible light photocatalytic activity for the hybrid $\text{MoS}_2/\text{anatase TiO}_2(001)$ nanocomposite: A first-principles study. <i>Chemical Physics Letters</i> , <b>2014</b> , 612, 285-288	2.5	21
10	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

9	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
8	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
7	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
6	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
5	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
4	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
3	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
2	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> , 2100378 <sup>3,5</sup>		0
1	Bimetallic Metal-Organic Framework with High-Adsorption Capacity toward Lithium Polysulfides for Lithium-Sulfur Batteries. <i>Energy and Environmental Materials</i> ,	13	15