

# Fei Xia

## List of Publications by Year in descending order

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65  
papers

1,943  
citations

304743

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265206

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67  
docs citations

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times ranked

2288  
citing authors

#	ARTICLE	IF	CITATIONS
1	Highly Fluorescent Polyimide Covalent Organic Nanosheets as Sensing Probes for the Detection of 2,4,6-Trinitrophenol. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 13415-13421.	8.0	234
2	Ubiquity and Diversity of Complete Ammonia Oxidizers (Comammox). <i>Applied and Environmental Microbiology</i> , 2018, 84, .	3.1	146
3	Origins of unique gold-catalysed chemo- and site-selective C-H functionalization of phenols with diazo compounds. <i>Chemical Science</i> , 2016, 7, 1988-1995.	7.4	118
4	Construction of unique six-coordinated titanium species with an organic amine ligand in titanasilicate and their unprecedented high efficiency for alkene epoxidation. <i>Chemical Communications</i> , 2015, 51, 9010-9013.	4.1	107
5	Enantioselective gold-catalyzed intermolecular [2+2] versus [4+2]-cycloadditions of 3-styrylindoles with N-allenamides: observation of interesting substituent effects. <i>Chemical Science</i> , 2015, 6, 5564-5570.	7.4	106
6	An Ylide Transformation of Rhodium(I) Carbene: Enantioselective Three-Component Reaction through Trapping of Rhodium(I)-Associated Ammonium Ylides by $\beta$ -Nitroacrylates. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 13136-13139.	13.8	90
7	Bond cleavage, fragment modification and reassembly in enantioselective three-component reactions. <i>Nature Communications</i> , 2015, 6, 5801.	12.8	86
8	Ras and GTPase-activating protein (GAP) drive GTP into a precatalytic state as revealed by combining FTIR and biomolecular simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 15295-15300.	7.1	75
9	DBU and DBU-Derived Ionic Liquid Synergistic Catalysts for the Conversion of Carbon Dioxide/Carbon Disulfide to $\alpha$ -Aryloxazolidinones/[1,3]Dithiolan $\alpha$ -ylidenephényl $\alpha$ -amine. <i>ChemCatChem</i> , 2016, 8, 830-838.	3.7	74
10	The Role of Magnesium for Geometry and Charge in GTP Hydrolysis, Revealed by Quantum Mechanics/Molecular Mechanics Simulations. <i>Biophysical Journal</i> , 2012, 103, 293-302.	0.5	46
11	DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: O-H Insertion versus C-H Insertion. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6485-6492.	2.5	45
12	Imidazolium ionic liquids/organic bases: Efficient intermolecular synergistic catalysts for the cycloaddition of CO <sub>2</sub> and epoxides under atmospheric pressure. <i>Molecular Catalysis</i> , 2018, 446, 124-130.	2.0	45
13	A Rh(II)-catalyzed multicomponent reaction by trapping an $\alpha$ -amino enol intermediate in a traditional two-component reaction pathway. <i>Science Advances</i> , 2017, 3, e1602467.	10.3	42
14	An improved protocol with a highly degenerate primer targeting copper-containing membrane-bound monooxygenase genes for community analysis of methane- and ammonia-oxidizing bacteria. <i>FEMS Microbiology Ecology</i> , 2017, 93, fiw244.	2.7	35
15	Co-catalysis over a bi-functional ligand-based Pd-catalyst for tandem bis-alkoxycarbonylation of terminal alkynes. <i>Green Chemistry</i> , 2018, 20, 2588-2595.	9.0	34
16	Detailed Structure of the H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> Guanosine Diphosphate Intermediate in Ras-GAP Decoded from FTIR Experiments by Biomolecular Simulations. <i>Journal of the American Chemical Society</i> , 2012, 134, 20041-20044.	13.7	33
17	Mechanistic Investigation of Aromatic C(sp <sup>2</sup> )-H and Alkyl C(sp <sup>3</sup> )-H Bond Insertion by Gold Carbenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1925-1932.	2.5	29
18	A DFT calculation-inspired Rh-catalyzed reaction via suppression of $\alpha$ -H shift in $\alpha$ -alkyldiazoacetates. <i>Chemical Science</i> , 2017, 8, 4312-4317.	7.4	28

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19	The specific vibrational modes of GTP in solution and bound to Ras: a detailed theoretical analysis by QM/MM simulations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21451.	2.8	27
20	Specific Substates of Ras To Interact with GAPs and Effectors: Revealed by Theoretical Simulations and FTIR Experiments. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1312-1317.	4.6	23
21	Highly Regioselective Radical Transformation of <i>N</i> -Sulfonyl-1,2,3-triazoles in Air. <i>Organic Letters</i> , 2019, 21, 6413-6417.	4.6	23
22	Relativistic density-functional study on the dehydrogenation reactivity of PtMCH <sub>2</sub> <sup>+</sup> (M=Cu,Ag,Au,Pt) toward NH <sub>3</sub> . <i>Chemical Physics Letters</i> , 2006, 418, 386-391.	2.6	22
23	Reaction mechanisms of carbon dioxide, ethylene oxide and amines catalyzed by ionic liquids BmimBr and BmimOAc: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27951-27957.	2.8	22
24	Mechanistic Studies of CO <sub>2</sub> Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. <i>Frontiers in Chemistry</i> , 2019, 7, 615.	3.6	20
25	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6678-6689.	5.3	20
26	Communities of ammonia oxidizers at different stages of <i>Spartina alterniflora</i> invasion in salt marshes of Yangtze River estuary. <i>Journal of Microbiology</i> , 2015, 53, 311-320.	2.8	19
27	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2091-2100.	5.3	19
28	Robust Heterogeneous Anisotropic Elastic Network Model Precisely Reproduces the Experimental B-factors of Biomolecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3704-3714.	5.3	18
29	A new algorithm for construction of coarse-grained sites of large biomolecules. <i>Journal of Computational Chemistry</i> , 2016, 37, 795-804.	3.3	18
30	Density Functional Characterization of Reactions of Bimetallic Carbenes PtMCH <sub>2</sub> <sup>+</sup> (M = Pt, Au) with NH <sub>3</sub> in the Gas Phase. <i>Organometallics</i> , 2005, 24, 1845-1851.	2.3	17
31	Base-Catalyzed Peptide Hydrolysis Is Insensitive to Mechanical Stress. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10126-10132.	2.6	17
32	Identifying essential pairwise interactions in elastic network model using the alpha shape theory. <i>Journal of Computational Chemistry</i> , 2014, 35, 1111-1121.	3.3	17
33	Minimum energy compact structures in force-quench polyubiquitin folding are domain swapped. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 6963-6968.	7.1	16
34	Multiscale Coarse-Graining via Normal Mode Analysis. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4797-4806.	5.3	16
35	DNA nanotweezers for stabilizing and dynamically lighting up a lipid raft on living cell membranes and the activation of T cells. <i>Chemical Science</i> , 2020, 11, 1581-1586.	7.4	16
36	CO <sub>2</sub> atmosphere enables efficient catalytic hydration of ethylene oxide by ionic liquids/organic bases at low water/epoxide ratios. <i>Green Chemistry</i> , 2021, 23, 3386-3391.	9.0	15

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37	Diastereoselective synthesis of 3,3-disubstituted 3-nitro-4-chromanone derivatives as potential antitumor agents. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1062-1066.	2.8	12
38	Ir-catalyzed tandem hydroformylation-transfer hydrogenation of olefins with (trans-/cis-)formic acid as hydrogen source in presence of 1,10-phenanthroline. <i>Journal of Catalysis</i> , 2020, 385, 183-193.	6.2	12
39	Conformational Features of Ras: Key Hydrogen-Bonding Interactions of Gln61 in the Intermediate State during GTP Hydrolysis. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8805-8813.	2.6	12
40	A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids. <i>RSC Advances</i> , 2017, 7, 51521-51527.	3.6	11
41	A triple-functionalised metal centre-catalyzed enantioselective multicomponent reaction. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2799-2804.	4.5	11
42	Construction of ultra-coarse-grained model of protein with a GÅ-like potential. <i>Chemical Physics Letters</i> , 2017, 681, 1-6.	2.6	10
43	Complete genome sequence of <i>Methylophilus</i> sp. TWE2 isolated from methane oxidation enrichment culture of tap-water. <i>Journal of Biotechnology</i> , 2015, 211, 121-122.	3.8	9
44	Deactivating Influence of 3-O-Glycosyl Substituent on Anomeric Reactivity of Thiomannoside Observed in Oligomannoside Synthesis. <i>Journal of Organic Chemistry</i> , 2017, 82, 2599-2621.	3.2	9
45	Determining Optimal Coarse-Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. <i>Journal of Computational Chemistry</i> , 2020, 41, 14-20.	3.3	9
46	Alcohol amine-catalyzed CO <sub>2</sub> conversion for the synthesis of quinoxaline-2,4-(1 <i>H</i> ,3 <i>H</i> )-dione in water. <i>RSC Advances</i> , 2020, 10, 34910-34915.	3.6	9
47	Identification of functional substates of KRas during GTP hydrolysis with enhanced sampling simulations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7653-7665.	2.8	9
48	Conformations and binding pockets of HRas and its guanine nucleotide exchange factors complexes in the guanosine triphosphate exchange process. <i>Journal of Computational Chemistry</i> , 2022, 43, 906-916.	3.3	9
49	Origins of Protons in H Bond Insertion Products of Phenols: Proton-Self-Sufficient Function via Water Molecules. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6523-6529.	2.5	8
50	Combined effect of confinement and affinity of crowded environment on conformation switching of adenylyate kinase. <i>Journal of Molecular Modeling</i> , 2014, 20, 2530.	1.8	7
51	Heterogeneous elastic network model improves description of slow motions of proteins in solution. <i>Chemical Physics Letters</i> , 2015, 618, 102-107.	2.6	7
52	Performance Comparison of Systematic Methods for Rigorous Definition of Coarse-Grained Sites of Large Biomolecules. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 214-222.	5.4	6
53	Combination of transition metal Rh-catalysis and tautomeric catalysis through a bi-functional ligand for one-pot tandem methoxycarbonylation-aminolysis of olefins towards primary amides. <i>Journal of Catalysis</i> , 2018, 361, 230-237.	6.2	6
54	A new method for the construction of coarse-grained models of large biomolecules from low-resolution cryo-electron microscopy data. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9720-9727.	2.8	6

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55	Coarse-Grained Simulation of Mechanical Properties of Single Microtubules With Micrometer Length. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 632122.	3.5	6
56	Reaction Mechanisms for C=O Bond Coupling from Pt <sub>4</sub> CH <sub>2</sub> <sup>+</sup> and O <sub>2</sub> : A Relativistic Density Functional Study. <i>Organometallics</i> , 2007, 26, 6076-6081.	2.3	5
57	How CuCl and CuCl <sub>2</sub> Insert into C=N Bonds of Diazo Compounds: An Electronic Structure and Mechanistic Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2029-2035.	2.5	5
58	Dual Functional Pd-Catalyzed Multicomponent Reaction by Umpolung Chemistry of the Oxygen Atom in Electrophiles. <i>Journal of Organic Chemistry</i> , 2021, 86, 6847-6854.	3.2	5
59	Ammonium promoting methane oxidation by stimulating the Type Ia methane-oxidizing bacteria in tidal flat sediments of the Yangtze River estuary. <i>Science of the Total Environment</i> , 2021, 793, 148470.	8.0	5
60	Accurate and Efficient Estimation of Lennard-Jones Interactions for Coarse-Grained Particles via a Potential Matching Method. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4879-4890.	5.3	5
61	Reaction Mechanism of CO <sub>2</sub> and Styrene Oxide Catalyzed by Ionic Liquids: A Combined DFT Calculation and Experimental Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7991-7998.	2.5	3
62	Conformer-related pathways in cycloaddition of vinylaziridines and alkynes catalyzed by rhodium(I)-complex. <i>Chemical Physics Letters</i> , 2018, 713, 21-25.	2.6	2
63	Electrostatic Polarization Effect on Cooperative Aggregation of Full Length Human Islet Amyloid. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1587-1595.	5.4	2
64	Iron speciation and annual records in black coral as new proxy for mining and environmental impacts. <i>Science of the Total Environment</i> , 2021, 776, 145965.	8.0	1
65	Tagged Highly Degenerate Primer (THDP)-PCR for Community Analysis of Methane- and Ammonia-oxidizing Bacteria Based on Copper-containing Membrane-bound Monooxygenases (CuMMO). <i>Bio-protocol</i> , 2017, 7, e2354.	0.4	0