Hong-Bin Xie

List of Publications by Year
in descending order

63	2,088	218592 26	265120 42
papers	citations	h-index	g-index

63	63	63	1774
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reaction Mechanism of Monoethanolamine with CO₂ in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	1.1	161
2	Superior Performance of Fe_{1â€“x}W_xO_{Î´} for the Selective Catalytic Reduction of NO_x with NH₃: Interaction between Fe and W. Environmental Science & Technology, 2016, 50, 13511-13519.	4.6	116
3	Atmospheric Fate of Monoethanolamine: Enhancing New Particle Formation of Sulfuric Acid as an Important Removal Process. Environmental Science & Technology, 2017, 51, 8422-8431.	4.6	95
4	Atmospheric Chemical Reactions of Monoethanolamine Initiated by OH Radical: Mechanistic and Kinetic Study. Environmental Science & Technology, 2014, 48, 1700-1706.	4.6	89
5	Effects of Atmospheric Water on Â·OH-initiated Oxidation of Organophosphate Flame Retardants: A DFT Investigation on TCPP. Environmental Science & Technology, 2017, 51, 5043-5051.	4.6	78
6	Predicting Gaseous Reaction Rates of Short Chain Chlorinated Paraffins with Â·OH: Overcoming the Difficulty in Experimental Determination. Environmental Science & Technology, 2014, 48, 13808-13816.	4.6	67
7	The role of carbonate in sulfamethoxazole degradation by peroxymonosulfate without catalyst and the generation of carbonate racial. Journal of Hazardous Materials, 2020, 398, 122827.	6.5	64
8	Photodegradation mechanism of sulfonamides with excited triplet state dissolved organic matter: A case of sulfadiazine with 4-carboxybenzophenone as a proxy. Journal of Hazardous Materials, 2015, 290, 9-15.	6.5	62
9	Deep learning for predicting toxicity of chemicals: a mini review. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 252-271.	2.9	61
10	Quantum Chemical Study on Â·Cl-Initiated Atmospheric Degradation of Monoethanolamine. Environmental Science & Technology, 2015, 49, 13246-13255.	4.6	58
11	Effective degradation of aqueous carbamazepine on a novel blue-colored TiO2 nanotube arrays membrane filter anode. Journal of Hazardous Materials, 2021, 402, 123530.	6.5	54
12	Highly-Dispersed Zinc Species on Zeolites for the Continuous and Selective Dehydrogenation of Ethane with CO₂ as a Soft Oxidant. ACS Catalysis, 2021, 11, 2819-2830.	5.5	53
13	Methanesulfonic Acid-driven New Particle Formation Enhanced by Monoethanolamine: A Computational Study. Environmental Science & Technology, 2019, 53, 14387-14397.	4.6	50
14	Atmospheric Oxidation of Piperazine Initiated by Â·Cl: Unexpected High Nitrosamine Yield. Environmental Science & Technology, 2018, 52, 9801-9809.	4.6	45
15	Mechanistic Understanding of Superoxide Radical-Mediated Degradation of Perfluorocarboxylic Acids. Environmental Science & Technology, 2022, 56, 624-633.	4.6	45
16	Piperazine Enhancing Sulfuric Acid-Based New Particle Formation: Implications for the Atmospheric Fate of Piperazine. Environmental Science & Technology, 2019, 53, 8785-8795.	4.6	41
17	Development of Prediction Models on Base-Catalyzed Hydrolysis Kinetics of Phthalate Esters with Density Functional Theory Calculation. Environmental Science & Technology, 2019, 53, 5828-5837.	4.6	41
18	A Computational Study of the Heats of Reaction of Substituted Monoethanolamine with CO₂. Journal of Physical Chemistry A, 2011, 115, 342-350.	1.1	40

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19	Theoretical Investigation on the Different Reaction Mechanisms of Aqueous 2-Amino-2-methyl-1-propanol and Monoethanolamine with CO₂. Industrial & Engineering Chemistry Research, 2014, 53, 3363-3372.	1.8	39
20	Prediction of Hydrolysis Pathways and Kinetics for Antibiotics under Environmental pH Conditions: A Quantum Chemical Study on Cephradine. Environmental Science & Technology, 2015, 49, 1552-1558.	4.6	39
21	Structural Effects of Amines in Enhancing Methanesulfonic Acid-Driven New Particle Formation. Environmental Science & Technology, 2020, 54, 13498-13508.	4.6	36
22	Acidâ€“Base Clusters during Atmospheric New Particle Formation in Urban Beijing. Environmental Science & Technology, 2021, 55, 10994-11005.	4.6	34
23	Anionic Phenolic Compounds Bind Stronger with Transthyretin than Their Neutral Forms: Nonnegligible Mechanisms in Virtual Screening of Endocrine Disrupting Chemicals. Chemical Research in Toxicology, 2013, 26, 1340-1347.	1.7	33
24	QSAR modeling for the ozonation of diverse organic compounds in water. Science of the Total Environment, 2020, 715, 136816.	3.9	33
25	Prediction Models on pK_a and Base-Catalyzed Hydrolysis Kinetics of Parabens: Experimental and Quantum Chemical Studies. Environmental Science & Technology, 2021, 55, 6022-6031.	4.6	31
26	Atmospheric chemical reactions of alternatives of polybrominated diphenyl ethers initiated by OH: A case study on triphenyl phosphate. Science of the Total Environment, 2016, 571, 1105-1114.	3.9	29
27	Kinetics and mechanism of OH-initiated atmospheric oxidation of organophosphorus plasticizers: A computational study on tri-p-cresyl phosphate. Chemosphere, 2018, 201, 557-563.	4.2	29
28	Different binding mechanisms of neutral and anionic poly-/perfluorinated chemicals to human transthyretin revealed by In silico models. Chemosphere, 2017, 182, 574-583.	4.2	28
29	Molecular understanding of the interaction of amino acids with sulfuric acid in the presence of water and the atmospheric implication. Chemosphere, 2018, 210, 215-223.	4.2	28
30	Computational Study of the Reactions of Chlorine Radicals with Atmospheric Organic Compounds Featuring NH_xâ€“Ï€-Bond (x = 1, 2) Structures. Journal of Physical Chemistry A, 2017, 121, 1657-1665.	1.1	27
31	Formation of Low-Volatile Products and Unexpected High Formaldehyde Yield from the Atmospheric Oxidation of Methylsiloxanes. Environmental Science & Technology, 2020, 54, 7136-7145.	4.6	27
32	Atmospheric oxidation mechanism and kinetics of isoprene initiated by chlorine radicals: A computational study. Science of the Total Environment, 2020, 712, 136330.	3.9	24
33	The degradation mechanism of sulfamethoxazole under ozonation: a DFT study. Environmental Sciences: Processes and Impacts, 2017, 19, 379-387.	1.7	23
34	Potential Application of Machine-Learning-Based Quantum Chemical Methods in Environmental Chemistry. Environmental Science & Technology, 2022, 56, 2115-2123.	4.6	22
35	Underlying mechanisms of reactive oxygen species and oxidative stress photoinduced by graphene and its surface-functionalized derivatives. Environmental Science: Nano, 2020, 7, 782-792.	2.2	21
36	Atmospheric Chemistry of Allylic Radicals from Isoprene: A Successive Cyclization-Driven Autoxidation Mechanism. Environmental Science & Technology, 2021, 55, 4399-4409.	4.6	20

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37	The role of organic acids in new particle formation from methanesulfonic acid and methylamine. Atmospheric Chemistry and Physics, 2022, 22, 2639-2650.	1.9	20
38	A molecular-scale study on the hydration of sulfuric acid-amide complexes and the atmospheric implication. Chemosphere, 2018, 213, 453-462.	4.2	18
39	Formation Mechanisms of Iodineâ€“Ammonia Clusters in Polluted Coastal Areas Unveiled by Thermodynamics and Kinetic Simulations. Environmental Science & Technology, 2020, 54, 9235-9242.	4.6	18
40	Atmospheric Autoxidation of Organophosphate Esters. Environmental Science & Technology, 2022, 56, 6944-6955.	4.6	18
41	Protonated sugars: vibrational spectroscopy and conformational structure of protonatedO-methyl Î±-D-galactopyranoside. Molecular Physics, 2012, 110, 1609-1615.	0.8	17
42	Computational Studies of Protonated Î²-d-Galactose and Its Hydrated Complex: Structures, Interactions, Proton Transfer Dynamics, and Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 4851-4859.	1.2	17
43	The Crucial Role of Skeleton Structure and Carbon Number on Short-Chain Alkane Activation over Zn/HZSM-5 Catalyst: An Experimental and Computational Study. Catalysis Letters, 2018, 148, 2069-2081.	1.4	17
44	Ferrate(<scp>vi</scp>) initiated oxidative degradation mechanisms clarified by DFT calculations: a case for sulfamethoxazole. Environmental Sciences: Processes and Impacts, 2017, 19, 370-378.	1.7	16
45	Adsorption of Nitrobenzene on the Surface of Ice: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2017, 121, 15746-15755.	1.5	16
46	Autoxidation mechanism for atmospheric oxidation of tertiary amines: Implications for secondary organic aerosol formation. Chemosphere, 2021, 273, 129207.	4.2	16
47	Heterogeneous Formation of HONO Catalyzed by CO₂. Environmental Science & Technology, 2021, 55, 12215-12222.	4.6	16
48	Theoretical study of the hydration effects on alkylamine and alkanolamine clusters and the atmospheric implication. Chemosphere, 2020, 243, 125323.	4.2	15
49	CO₂ Absorption in an Alcoholic Solution of Heavily Hindered Alkanolamine: Reaction Mechanism of 2-(tert-Butylamino)ethanol with CO₂ Revisited. Journal of Physical Chemistry A, 2015, 119, 6346-6353.	1.1	14
50	Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenylâ€based organic pollutants. International Journal of Quantum Chemistry, 2018, 118, e25533.	1.0	14
51	Transformation pathways of MeO-PBDEs catalyzed by active center of P450 enzymes: A DFT investigation employing 6-MeO-BDE-47 as a case. Chemosphere, 2015, 120, 631-636.	4.2	13
52	Amine-Enhanced Methanesulfonic Acid-Driven Nucleation: Predictive Model and Cluster Formation Mechanism. Environmental Science & Technology, 2022, 56, 7751-7760.	4.6	13
53	Tri-Base Synergy in Sulfuric Acid-Base Clusters. Atmosphere, 2021, 12, 1260.	1.0	12
54	Toward rational design of amines for CO2 capture: Substituent effect on kinetic process for the reaction of monoethanolamine with CO2. Journal of Environmental Sciences, 2015, 37, 75-82.	3.2	11

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55	Atmospheric chemical reaction mechanism and kinetics of 1,2-bis(2,4,6-tribromophenoxy)ethane initiated by OH radical: a computational study. RSC Advances, 2017, 7, 9484-9494.	1.7	11
56	Grand canonical Monte Carlo simulation on adsorption of aniline on the ice surface. Journal of Molecular Liquids, 2019, 290, 111221.	2.3	11
57	Role of hydrogen bond capacity of solvents in reactions of amines with CO2: A computational study. Journal of Environmental Sciences, 2020, 91, 271-278.	3.2	11
58	Computational investigation of the nitrosation mechanism of piperazine in CO2 capture. Chemosphere, 2017, 186, 341-349.	4.2	10
59	Mechanism and predictive model development of reaction rate constants for N-center radicals with O2. Chemosphere, 2019, 237, 124411.	4.2	8
60	Interaction and reaction of the hydroxyl ion with Î²-d-galactose and its hydrated complex: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 12086.	1.3	5
61	Organic acid-ammonia ion-induced nucleation pathways unveiled by quantum chemical calculation and kinetics modeling: A case study of 3-methyl-1,2,3-butanetricarboxylic acid. Chemosphere, 2021, 284, 131354.	4.2	4
62	Quantum chemical simulations revealed the toxicokinetic mechanisms of organic phosphorus flame retardants catalyzed by P450 enzymes. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 272-291.	2.9	2
63	Response to Comment on â€œMechanistic Understanding of Superoxide Radical-Mediated Degradation of Perfluorocarboxylic Acidsâ€• Environmental Science & Technology, 2022, 56, 5289-5291.	4.6	2