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	Atmospheric Autoxidation of Organophosphate Esters. Environmental Science & Technology, 2022, 56, 6944-6955.	4.6	18
2	Potential Application of Machine-Learning-Based Quantum Chemical Methods in Environmental Chemistry. Environmental Science & Technology, 2022, 56, 2115-2123.	4.6	22
3	Mechanistic Understanding of Superoxide Radical-Mediated Degradation of Perfluorocarboxylic Acids. Environmental Science & Technology, 2022, 56, 624-633.	4.6	45
4	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
5	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
6	Amine-Enhanced Methanesulfonic Acid-Driven Nucleation: Predictive Model and Cluster Formation Mechanism. Environmental Science & Technology, 2022, 56, 7751-7760.	4.6	13
7	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
8	Autoxidation mechanism for atmospheric oxidation of tertiary amines: Implications for secondary organic aerosol formation. Chemosphere, 2021, 273, 129207.	4.2	16
9	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
10	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
11	Atmospheric Chemistry of Allylic Radicals from Isoprene: A Successive Cyclization-Driven Autoxidation Mechanism. Environmental Science & Technology, 2021, 55, 4399-4409.	4.6	20
12	Heterogeneous Formation of HONO Catalyzed by CO₂. Environmental Science & Technology, 2021, 55, 12215-12222.	4.6	16
13	Acidâ€“Base Clusters during Atmospheric New Particle Formation in Urban Beijing. Environmental Science & Technology, 2021, 55, 10994-11005.	4.6	34
14	Tri-Base Synergy in Sulfuric Acid-Base Clusters. Atmosphere, 2021, 12, 1260.	1.0	12
15	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
16	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
17	Theoretical study of the hydration effects on alkylamine and alkanolamine clusters and the atmospheric implication. Chemosphere, 2020, 243, 125323.	4.2	15
18	Structural Effects of Amines in Enhancing Methanesulfonic Acid-Driven New Particle Formation. Environmental Science & Technology, 2020, 54, 13498-13508.	4.6	36

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19	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
20	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
21	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
22	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
23	QSAR modeling for the ozonation of diverse organic compounds in water. Science of the Total Environment, 2020, 715, 136816.	3.9	33
24	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
25	Mechanism and predictive model development of reaction rate constants for N-center radicals with O2. Chemosphere, 2019, 237, 124411.	4.2	8
26	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
27	Methanesulfonic Acid-driven New Particle Formation Enhanced by Monoethanolamine: A Computational Study. Environmental Science & Technology, 2019, 53, 14387-14397.	4.6	50
28	Grand canonical Monte Carlo simulation on adsorption of aniline on the ice surface. Journal of Molecular Liquids, 2019, 290, 111221.	2.3	11
29	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
30	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
31	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
32	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
33	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
34	A molecular-scale study on the hydration of sulfuric acid-amide complexes and the atmospheric implication. Chemosphere, 2018, 213, 453-462.	4.2	18
35	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
36	Atmospheric Oxidation of Piperazine Initiated by Â·Cl: Unexpected High Nitrosamine Yield. Environmental Science & Technology, 2018, 52, 9801-9809.	4.6	45

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37	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
38	The degradation mechanism of sulfamethoxazole under ozonation: a DFT study. Environmental Sciences: Processes and Impacts, 2017, 19, 379-387.	1.7	23
39	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
40	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
41	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
42	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
43	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
44	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
45	Computational investigation of the nitrosation mechanism of piperazine in CO2 capture. Chemosphere, 2017, 186, 341-349.	4.2	10
46	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
47	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
48	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
49	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
50	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
51	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
52	Quantum Chemical Study on Â·Cl-Initiated Atmospheric Degradation of Monoethanolamine. Environmental Science & Technology, 2015, 49, 13246-13255.	4.6	58
53	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
54	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

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55	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
56	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
57	Atmospheric Chemical Reactions of Monoethanolamine Initiated by OH Radical: Mechanistic and Kinetic Study. Environmental Science & Technology, 2014, 48, 1700-1706.	4.6	89
58	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
59	Protonated sugars: vibrational spectroscopy and conformational structure of protonatedO-methyl Î±-D-galactopyranoside. Molecular Physics, 2012, 110, 1609-1615.	0.8	17
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	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
62	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
63	Reaction Mechanism of Monoethanolamine with CO₂ in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	1.1	161