Ju Xie

List of Publications by Year
in descending order

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61	966	516215 16	525886 27
papers	citations	h-index	g-index

61	61	61	1013
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unravelling the effects of complexation of transition metal ions on the hydroxylation of catechol over the whole pH region. Journal of Environmental Sciences, 2022, 115, 392-402.	3.2	7
2	Theoretical insights into the degradation of swep by hydroxyl radicals in atmosphere and water environment: Mechanisms, kinetics and toxicity. Science of the Total Environment, 2022, 816, 151651.	3.9	3
3	[Mo₃S₁₃]^{2â^'}as bidirectional cluster catalysts for high-performance Liâ€“S batteries. Catalysis Science and Technology, 2022, 12, 3431-3435.	2.1	6
4	Reactivity of aromatic contaminants towards nitrate radical in tropospheric gas and aqueous phase. Journal of Hazardous Materials, 2021, 401, 123396.	6.5	9
5	Theoretical study on a kind of cyclization mechanism of boron trichloride and hexamethyldisilazane to form the borazine ring for SiBCN ceramics precursor. Ceramics International, 2021, 47, 6068-6076.	2.3	2
6	Heteroatom-bridged pillar[4]quinone: evolutionary active cathode material for lithium-ion battery using density functional theory. Journal of Chemical Sciences, 2021, 133, 1.	0.7	11
7	Degradation mechanisms, kinetics and eco-toxicity assessment of 2,4-Dinitrophenol by oxygen-containing free radicals in aqueous solution. Molecular Physics, 2021, 119, e1886365.	0.8	6
8	Full insights into the roles of pH on hydroxylation of aromatic acids/bases and toxicity evaluation. Water Research, 2021, 190, 116689.	5.3	22
9	Adsorption of [<scp>BF₄</scp>]^{â^'} anionâ€based ionic liquids on phosphorene, arsenene, and antimonene: A density functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26668.	1.0	3
10	Theoretical prediction on photoelectric and supramolecular properties of benzoquinone-tetrathiafulvalene macrocyclic molecules. Journal of Molecular Modeling, 2021, 27, 157.	0.8	1
11	The roles of HOâ€¢, ClOâ€¢ and BrOâ€¢ radicals in caffeine degradation: A theoretical study. Science of the Total Environment, 2021, 768, 144733.	3.9	31
12	Self-Assembled Polyoxometalate Nanodots as Bidirectional Cluster Catalysts for Polysulfide/Sulfide Redox Conversion in Lithiumâ€“Sulfur Batteries. ACS Nano, 2021, 15, 12222-12236.	7.3	77
13	Ozonolysis of Permethrin in the Atmosphere: Mechanism, Kinetics, and Evaluation of Toxicity. Journal of Physical Chemistry A, 2021, 125, 7705-7715.	1.1	9
14	Embedding Cobalt Atom Clusters in CNTâ€Wired MoS₂ Tubeâ€inâ€Tube Nanostructures with Enhanced Sulfur Immobilization and Catalyzation for Liâ€“S Batteries. Small, 2021, 17, e2102710.	5.2	52
15	Acetaminophen degradation by hydroxyl and organic radicals in the peracetic acid-based advanced oxidation processes: Theoretical calculation and toxicity assessment. Journal of Hazardous Materials, 2021, 416, 126250.	6.5	17
16	Atmospheric ozonolysis of crotonaldehyde in the absence and presence of hydroxylated silica oligomer cluster adsorption. Chemosphere, 2021, 281, 130996.	4.2	4
17	Construction of Polyfunctionalized 2,4-Dioxa-8-azaspiro[5.5]undec-9-enes and 2,4,8-Triazaspiro[5.5]undec-9-enes via a Domino [2+2+2] Cycloaddition Reaction. Journal of Organic Chemistry, 2021, 86, 1827-1842.	1.7	12
18	Inorganicâ€“organic hybrid supramolecular architectures based on Keggin polyoxometalates and crown ether: synthesis, crystal structure and electrochemical properties. CrystEngComm, 2021, 23, 8482-8489.	1.3	14

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19	Theoretical Study on the Mechanism of the Initial Ammonolysis Reactions of the Main Raw Materials for the Formation of SiBCN Ceramics. ChemistrySelect, 2021, 6, 12233-12245.	0.7	0
20	4-Pentenoyl-isoleucyl-chitosan oligosaccharide and acrylamide functional monomer-dependent hybrid bilayer molecularly imprinted membrane for sensitive electrochemical sensing of bisphenol A. RSC Advances, 2021, 11, 36769-36776.	1.7	5
21	Theoretical prediction of structures and inclusion properties of heteroatom-bridged pillar[n]arenes. Structural Chemistry, 2020, 31, 329-337.	1.0	9
22	Theoretical insight into the degradation of p-nitrophenol by OH radicals synergized with other active oxidants in aqueous solution. Journal of Hazardous Materials, 2020, 389, 121901.	6.5	62
23	Pillar[5]arene-based [3]rotaxanes: Convenient construction via multicomponent reaction and pH responsive self-assembly in water. Chinese Chemical Letters, 2020, 31, 1550-1553.	4.8	18
24	Theoretical investigation on the contribution of HO , SO4- and CO3- radicals to the degradation of phenacetin in water: Mechanisms, kinetics, and toxicity evaluation. Ecotoxicology and Environmental Safety, 2020, 204, 110977.	2.9	18
25	Highly Efficient Dehydrogenation of 2,3-Butanediol Induced by Metalâ€“Support Interface over Cu-SiO₂ Catalysts. ACS Sustainable Chemistry and Engineering, 2020, 8, 15716-15731.	3.2	18
26	Composite polymerized molecular imprinting membrane-based electrochemical sensor for sensitive determination of curcumin by using 4-pentenoyl-aminoacyl-chitosan oligosaccharide as functional monomer oligomer. Journal of Electroanalytical Chemistry, 2020, 879, 114793.	1.9	18
27	Theoretical Study of Ozonation of Methylparaben and Ethylparaben in Aqueous Solution. Journal of Physical Chemistry A, 2020, 124, 10967-10976.	1.1	3
28	Ozonation of diclofenac in the aqueous solution: Mechanism, kinetics and ecotoxicity assessment. Environmental Research, 2020, 188, 109713.	3.7	19
29	Effect of pH on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mo linebreak="goodbreak" linebreakstyle="after">Â·</mml:mo><mml:mi>O</mml:mi><mml:mi>H</mml:mi></mml:mrow></mml:math>-induced degradation progress of syringol/syringaldehyde and health effect. Chemosphere, 2020, 255, 126893.	4.2	15
30	Bimetallic sulfide Co8FeS8/Nâ€“C dodecahedral nanocages via cation exchange as counter electrode for dye-sensitized solar cells. Journal of Alloys and Compounds, 2020, 829, 154526.	2.8	15
31	H-bond catalytic mechanism of aromatic electrophilic substitution between phenol and formaldehyde. Tetrahedron, 2020, 76, 131055.	1.0	0
32	Degradation of prosulfocarb by hydroxyl radicals in gas and aqueous phase: Mechanisms, kinetics and toxicity. Ecotoxicology and Environmental Safety, 2020, 191, 110175.	2.9	15
33	Template-assisted synthesis of LiNi0.8Co0.15Al0.05O2 hollow nanospheres as cathode material for lithium ion batteries. Journal of Materials Science, 2020, 55, 9493-9503.	1.7	6
34	Gaseous and heterogeneous reactions of low-molecular-weight (LMW) unsaturated ketones with O3: Mechanisms, kinetics, and effects of mineral dust in tropospheric chemical processes. Chemical Engineering Journal, 2020, 395, 125083.	6.6	27
35	Solubility of Acetoguanamine in Twelve Neat Solvents from 283.15 to 323.15 K. Journal of Chemical & Engineering Data, 2019, 64, 4546-4550.	1.0	2
36	Self-Assembled Supramolecular Polyoxometalate Hybrid Architecture as a Multifunctional Oxidation Catalyst. ACS Applied Materials & Interfaces, 2019, 11, 38708-38718.	4.0	38

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37	Water determines the products: an unexpected BrÃ¸nsted acid-catalyzed POâ€“R cleavage of P(<scp>iii</scp>) esters selectively producing P(O)â€“H and P(O)â€“R compounds. Green Chemistry, 2019, 21, 2916-2922.	4.6	18
38	Mechanisms and Kinetic Parameters for the Gas-Phase Reactions of 3-Methyl-3-buten-2-one and 3-Methyl-3-penten-2-one with Ozone. Journal of Physical Chemistry A, 2019, 123, 2745-2755.	1.1	11
39	Density functional theory study of selective aerobic oxidation of cyclohexane: the roles of acetic acid and cobalt ion. Journal of Molecular Modeling, 2019, 25, 71.	0.8	11
40	Highly Selective and Efficient Reduction of CO₂ to Methane by Activated Alkaline Earth Metal Hydrides without a Catalyst. ACS Sustainable Chemistry and Engineering, 2019, 7, 4831-4841.	3.2	17
41	Bidirectional heterostructures consisting of graphene and lateral MoS₂/WS₂ composites: a first-principles study. RSC Advances, 2019, 9, 34986-34994.	1.7	4
42	Development of the Visibleâ€Light Response of CeO_{2â¯x} with a high Ce³⁺ Content and Its Photocatalytic Properties. ChemCatChem, 2018, 10, 1267-1271.	1.8	37
43	Electroic and optical properties of germanene/MoS2 heterobilayers: first principles study. Journal of Molecular Modeling, 2018, 24, 333.	0.8	12
44	Theoretical study on host-guest interaction between pillar[4]arene and molecules or ions. Journal of Molecular Modeling, 2018, 24, 199.	0.8	10
45	Controllable Supramolecular Chiral Twisted Nanoribbons from Achiral Conjugated Oligoaniline Derivatives. Journal of the American Chemical Society, 2018, 140, 9417-9425.	6.6	62
46	Computational electrochemistry of Pillar[5]quinone cathode material for lithium-ion batteries. Computational Materials Science, 2017, 137, 233-242.	1.4	17
47	Theoretical investigation of pillar[4]quinone as a cathode active material for lithium-ion batteries. Journal of Molecular Modeling, 2017, 23, 105.	0.8	14
48	A new precursor to synthesize g-C₃N₄ with superior visible light absorption for photocatalytic application. Catalysis Science and Technology, 2017, 7, 1826-1830.	2.1	35
49	Cyclodimerization of 3-phenacylideneoxindolines with amino esters for the synthesis of dispiro[indoline-3,1â€²-cyclopentane-3â€²,3â€³-indolines]. Heterocyclic Communications, 2017, 23, 297-303.	0.6	2
50	Ionic S_Niâ€Si Nucleophilic Substitution in Nâ€Methylanilineâ€Induced Siâ¯Si Bond Cleavages of Si₂Cl₆. Chemistry - A European Journal, 2016, 22, 5010-5016.	1.7	10
51	Theoretical study of a novel imino bridged pillar[5]arene derivative. Chemical Physics Letters, 2016, 662, 25-30.	1.2	10
52	New cytotoxic trichothecene macrolide epimers from endophytic Myrothecium roridum IFB-E012. Journal of Antibiotics, 2016, 69, 652-655.	1.0	10
53	Formation of a series of stable pillar[5]arene-based pseudo[1]-rotaxanes and their [1]rotaxanes in the crystal state. Scientific Reports, 2016, 6, 28748.	1.6	40
54	Molecular diversity of the three-component reaction of Î±-amino acids, dialkyl acetylenedicarboxylates and N-substituted maleimides. Organic and Biomolecular Chemistry, 2016, 14, 6497-6507.	1.5	25

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55	Computational simulation study on the anion recognition properties of functionalized tetraphenyl porphyrins. Journal of Molecular Modeling, 2015, 21, 140.	0.8	4
56	Specific binding and inhibition of 6-benzylaminopurine to catalase: Multiple spectroscopic methods combined with molecular docking study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 327-335.	2.0	23
57	Theoretical study on halide anion recognitions by pyrrole- and benzene-strapped calix[4]pyrroles. Computational and Theoretical Chemistry, 2013, 1007, 1-8.	1.1	3
58	Theoretical study on the ionâ€“pair recognition of Na+/Xâˆ’Â(XÂ=ÂFâˆ’Â, Clâˆ’Â, Brâˆ’Â) by urea calix[4]bis crown-3 derivative. Molecular Simulation, 2013, 39, 621-628.	0.9	2
59	Theoretical study on ion-pair recognition of M+X- (M = Li, Na, K and X = F, Cl, Br) by formylaminocalix[4]arene derivatives. Journal of Molecular Modeling, 2012, 18, 4985-4993.	0.8	2
60	Cycloaddition reactions of N-heterocyclic stable silylenes with ethylene andÂformaldehyde. Journal of Organometallic Chemistry, 2011, 696, 841-845.	0.8	2
61	Theoretical study of solvent effects on the structures and isomerization of silylenoid H2SiLiF. Structural Chemistry, 2007, 18, 65-70.	1.0	11