Yong Dong Liu

List of Publications by Year
in descending order

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32 papers	363 citations	933447 10 h-index	839539 18 g-index
32 all docs	32 docs citations	32 times ranked	433 citing authors

#	Article	IF	Citations
1	Formation Mechanism of NDMA from Ranitidine, Trimethylamine, and Other Tertiary Amines during Chloramination: A Computational Study. Environmental Science & Technology, 2014, 48, 8653-8663.	10.0	72
2	Prediction on the mutagenicity of nitroaromatic compounds using quantum chemistry descriptors based QSAR and machine learning derived classification methods. Ecotoxicology and Environmental Safety, 2019, 186, 109822.	6.0	39
3	In vivo toxicity of nitroaromatic compounds to rats: QSTR modelling and interspecies toxicity relationship with mouse. Journal of Hazardous Materials, 2020, 399, 122981.	12.4	31
4	Comparison of N-nitrosodimethylamine formation mechanisms from dimethylamine during chloramination and ozonation: A computational study. Journal of Hazardous Materials, 2017, 321, 362-370.	12.4	26
5	Theoretical studies on the formation of N-nitrosodimethylamine. Computational and Theoretical Chemistry, 2007, 802, 1-6.	1.5	23
6	Development of a Biomimetic Chondroitin Sulfate-modified Hydrogel to Enhance the Metastasis of Tumor Cells. Scientific Reports, 2016, 6, 29858.	3.3	20
7	Degradation Mechanisms and Substituent Effects of N-Chloro-Î±-Amino Acids: A Computational Study. Environmental Science & Technology, 2020, 54, 2635-2645.	10.0	18
8	Theoretical investigation of the isomerization of N2O3 and the N-nitrosation of dimethylamine by asym-N2O3, sym-N2O3, and transâ€“cis N2O3 isomers. Computational and Theoretical Chemistry, 2009, 908, 107-113.	1.5	15
9	Formation mechanism of chloropicrin from amines and free amino acids during chlorination: A combined computational and experimental study. Journal of Hazardous Materials, 2021, 416, 125819.	12.4	13
10	NDMA formation mechanisms from typical hydrazines and hydrazones during ozonation: A computational study. Journal of Hazardous Materials, 2019, 366, 370-377.	12.4	12
11	Does the metalâ€“metal sextuple bond exist in the bimetallic sandwich compounds Cr₂(C₆H₆)₂, Mo₂(C₆H₆)₂, and W₂(C₆H₆)₂?^{â€}. Molecular Physics, 2013, 111, 2523-2535.	1.7	11
12	Structureâ€“activity relationship of nitrosating agents in the nitrosation reactions of ammonia: a theoretical study. Theoretical Chemistry Accounts, 2009, 124, 261-268.	1.4	9
13	Theoretical investigation of reactivities of amines in the N-nitrosation reactions by N2O3. Journal of Molecular Modeling, 2011, 17, 669-680.	1.8	9
14	The formation mechanism of chloropicrin from methylamine during chlorination: a DFT study. Environmental Sciences: Processes and Impacts, 2019, 21, 761-770.	3.5	9
15	Iron(II) porphyrins induced conversion of nitrite into nitric oxide: A computational study. Journal of Inorganic Biochemistry, 2015, 150, 126-132.	3.5	7
16	THEORETICAL STUDY ON INTERNAL ROTATION OF NITROSOUREAS AND TOXICOLOGICAL ANALYSIS. Journal of Theoretical and Computational Chemistry, 2007, 06, 245-253.	1.8	6
17	The reactions of Cr(CO)₆, Fe(CO)₅, and Ni(CO)₄ with O₂ yield viable oxoâ€metal carbonyls. Journal of Computational Chemistry, 2014, 35, 998-1009.	3.3	6
18	Degradation mechanisms of simple aliphatic amines under ozonation: a DFT study. Environmental Sciences: Processes and Impacts, 2021, 23, 480-490.	3.5	6

#	Article	IF	Citations
19	Theoretical investigation of mono- and bi-function alkylating agents transformed from nitrosodimethylamine derivatives. Computational and Theoretical Chemistry, 2009, 893, 106-110.	1.5	5
20	The Influence of Phosphate Buffer on the Formation of N-Nitrosodimethylamine from Dimethylamine Nitrosation. Journal of Chemistry, 2013, 2013, 1-9.	1.9	4
21	Theoretical Investigation of the Gas-Phase S_N2 Reactions of Anionic and Neutral Nucleophiles with Chloramines. Journal of Physical Chemistry A, 2018, 122, 3045-3056.	2.5	4
22	Reaction Mechanisms of Histidine and Carnosine with Hypochlorous Acid Along with Chlorination Reactivity of N-Chlorinated Intermediates: A Computational Study. Chemical Research in Toxicology, 2022, 35, 750-759.	3.3	4
23	Theoretical investigation of the decomposition mechanisms of N-(2-chloroethyl)-N-nitrosourea. Theoretical Chemistry Accounts, 2007, 118, 973-978.	1.4	3
24	Reinvestigation of NDMA formation mechanisms from tertiary amines during chloramination: a DFT study. Environmental Science: Water Research and Technology, 2020, 6, 2078-2088.	2.4	3
25	1,1â€Dilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure. ChemPhysChem, 2016, 17, 1623-1629.	2.1	2
26	Transformation mechanisms of acetaldehyde and its substituted aldehydes into the corresponding nitriles and (N-chloro)amides during chloramination: A computational study. Science of the Total Environment, 2022, 836, 155592.	8.0	2
27	Theoretical Investigation of N-Nitrosation Mechanism of Amino Acids Mediated by N2O3. , 2009, , .		1
28	Theoretical investigation of the isomerization and dissociation reactions of all the HOONO2 isomers. Computational and Theoretical Chemistry, 2010, 959, 42-48.	1.5	1
29	Effects of heavy metal ions on N-nitrosodimethylamine (NDMA) formation. RSC Advances, 2016, 6, 70474-70479.	3.6	1
30	Experimental and Theoretical Investigation of Effects of Ethanol and Acetic Acid on Carcinogenic NDMA Formation in Simulated Gastric Fluid. Journal of Physical Chemistry A, 2016, 120, 4505-4513.	2.5	1
31	Notice of Retraction: A Comparative Investigation of the Nitrosodimethylamine Formation from the Nitrosation of Dimethylamine and Trimethylamine by Nitrite under the Neutral Condition. , 2011, , .		0
32	Prototypical metalâ€“oxo bonds: the reactions of Cr(PF3)6, Fe(PF3)5, and Ni(PF3)4 with oxygen. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	0