# 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | Degradation mechanisms of simple aliphatic amines under ozonation: a DFT study. Environmental Sciences: Processes and Impacts, 2021, 23, 480-490. | 3.5 | 6 |
| 5 | 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 |
| 6 | 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 |
| 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 | 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 |
| 9 | The formation mechanism of chloropicrin from methylamine during chlorination: a DFT study. Environmental Sciences: Processes and Impacts, 2019, 21, 761-770. | 3.5 | 9 |
| 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 | Theoretical Investigation of the Gas-Phase S<sub>N</sub>2 Reactions of Anionic and Neutral Nucleophiles with Chloramines. Journal of Physical Chemistry A, 2018, 122, 3045-3056. | 2.5 | 4 |
| 12 | 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 |
| 13 | 1,1â€Ðilithioethylene: Toward Spectroscopic Identification of the Definitive Singlet Ground Electronic State of a Peculiar Structure. ChemPhysChem, 2016, 17, 1623-1629. | 2.1 | 2 |
| 14 | Effects of heavy metal ions on N-nitrosodimethylamine (NDMA) formation. RSC Advances, 2016, 6, 70474-70479. | 3.6 | 1 |
| 15 | Development of a Biomimetic Chondroitin Sulfate-modified Hydrogel to Enhance the Metastasis of Tumor Cells. Scientific Reports, 2016, 6, 29858. | 3.3 | 20 |
| 16 | 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 |
| 17 | Iron(II) porphyrins induced conversion of nitrite into nitric oxide: A computational study. Journal of Inorganic Biochemistry, 2015, 150, 126-132. | 3.5 | 7 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | The reactions of Cr(CO)<sub>6</sub>, Fe(CO)<sub>5</sub>, and Ni(CO)<sub>4</sub> with O<sub>2</sub> yield viable oxoâ€metal carbonyls. Journal of Computational Chemistry, 2014, 35, 998-1009. | 3.3 | 6 |
| 20 | 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 |
| 21 | Does the metalâ€"metal sextuple bond exist in the bimetallic sandwich compounds Cr<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>, Mo<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>, and W<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>?<sup>â€</sup>. Molecular Physics, 2013, 111, 2523-2535. | 1.7 | 11 |
| 22 | The Influence of Phosphate Buffer on the Formation of N-Nitrosodimethylamine from Dimethylamine Nitrosation. Journal of Chemistry, 2013, 2013, 1-9. | 1.9 | 4 |
| 23 | Theoretical investigation of reactivities of amines in the N-nitrosation reactions by N2O3. Journal of Molecular Modeling, 2011, 17, 669-680. | 1.8 | 9 |
| 24 | 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 |
| 25 | Theoretical investigation of the isomerization and dissociation reactions of all the HOONO2 isomers. Computational and Theoretical Chemistry, 2010, 959, 42-48. | 1.5 | 1 |
| 26 | Theoretical Investigation of N-Nitrosation Mechanism of Amino Acids Mediated by N2O3. , 2009, , . | | 1 |
| 27 | Theoretical investigation of mono- and bi-function alkylating agents transformed from nitrosodimethylamine derivatives. Computational and Theoretical Chemistry, 2009, 893, 106-110. | 1.5 | 5 |
| 28 | 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 |
| 29 | 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 |
| 30 | THEORETICAL STUDY ON INTERNAL ROTATION OF NITROSOUREAS AND TOXICOLOGICAL ANALYSIS. Journal of Theoretical and Computational Chemistry, 2007, 06, 245-253. | 1.8 | 6 |
| 31 | Theoretical studies on the formation of N-nitrosodimethylamine. Computational and Theoretical Chemistry, 2007, 802, 1-6. | 1.5 | 23 |
| 32 | Theoretical investigation of the decomposition mechanisms of N-(2-chloroethyl)-N-nitrosourea. Theoretical Chemistry Accounts, 2007, 118, 973-978. | 1.4 | 3 |