# Hujun Xie

## List of Publications by Year in descending order



| | | | |
|---|---|---|---|
| 139 papers | 3,097 citations | 172207 29 h-index | 223531 46 g-index |
| 146 all docs | 146 docs citations | 146 times ranked | 2858 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Fabrication of ovalbumin/Î²-carrageenan complex nanoparticles as a novel carrier for curcumin delivery. Food Hydrocolloids, 2019, 89, 111-121. | 5.6 | 120 |
| 2 | Development of ovalbumin-pectin nanocomplexes for vitamin D3 encapsulation: Enhanced storage stability and sustained release in simulated gastrointestinal digestion. Food Hydrocolloids, 2020, 106, 105926. | 5.6 | 112 |
| 3 | Selective Synthesis of Osmanaphthalene and Osmanaphthalyne by Intramolecular Cï£¿H Activation. Angewandte Chemie - International Edition, 2009, 48, 5461-5464. | 7.2 | 106 |
| 4 | Highly transparent, self-healing conductive elastomers enabled by synergistic hydrogen bonding interactions. Chemical Engineering Journal, 2020, 393, 124685. | 6.6 | 98 |
| 5 | Osmapyridine and Osmapyridinium from a Formal [4+2] Cycloaddition Reaction. Angewandte Chemie - International Edition, 2009, 48, 5430-5434. | 7.2 | 92 |
| 6 | Explore the interaction mechanism between zein and EGCG using multi-spectroscopy and molecular dynamics simulation methods. Food Hydrocolloids, 2021, 120, 106906. | 5.6 | 89 |
| 7 | Development of antifungal gelatin-based nanocomposite films functionalized with natamycin-loaded zein/casein nanoparticles. Food Hydrocolloids, 2021, 113, 106506. | 5.6 | 72 |
| 8 | Preparation of Î²-lactoglobulin/gum arabic complex nanoparticles for encapsulation and controlled release of EGCG in simulated gastrointestinal digestion model. Food Chemistry, 2021, 354, 129516. | 4.2 | 69 |
| 9 | Curcumin-loaded core-shell biopolymer nanoparticles produced by the pH-driven method: Physicochemical and release properties. Food Chemistry, 2021, 355, 129686. | 4.2 | 69 |
| 10 | Isolation, purification, and antioxidant activities of degraded polysaccharides from Enteromorpha prolifera. International Journal of Biological Macromolecules, 2015, 81, 1026-1030. | 3.6 | 66 |
| 11 | Mechanisms and Origins of Switchable Regioselectivity of Palladium- and Nickel-Catalyzed Allene Hydrosilylation with N-Heterocyclic Carbene Ligands: Â Theoretical Study. Journal of Organic Chemistry, 2014, 79, 4517-4527. | 1.7 | 57 |
| 12 | Iron-Catalyzed Enantioselective Siâ€“H Bond Insertions. Organic Letters, 2018, 20, 6544-6549. | 2.4 | 56 |
| 13 | Spirooxindole synthesis via palladium-catalyzed dearomative reductive-Heck reaction. Organic and Biomolecular Chemistry, 2017, 15, 2711-2715. | 1.5 | 55 |
| 14 | Fabrication of Zein-Lecithin-EGCG complex nanoparticles: Characterization, controlled release in simulated gastrointestinal digestion. Food Chemistry, 2021, 365, 130542. | 4.2 | 55 |
| 15 | Controllable hierarchical self-assembly of porphyrin-derived supra-amphiphiles. Nature Communications, 2019, 10, 1399. | 5.8 | 51 |
| 16 | Application of whey protein isolate fibrils in encapsulation and protection of Î²-carotene. Food Chemistry, 2021, 346, 128963. | 4.2 | 49 |
| 17 | Visibleâ€Light Promoted Distereodivergent Intramolecular Oxyamidation of Alkenes. Chemistry - A European Journal, 2016, 22, 18695-18699. | 1.7 | 44 |
| 18 | The regulation of sodium alginate on the stability of ovalbumin-pectin complexes for VD3 encapsulation and in vitro simulated gastrointestinal digestion study. Food Research International, 2021, 140, 110011. | 2.9 | 41 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Chameleon-like Behavior of the Directing Group in the Rh(III)-Catalyzed Regioselective Câ€“H Amidation of Indole: An Experimental and Computational Study. ACS Catalysis, 2019, 9, 10233-10244. | 5.5 | 40 |
| 20 | [3+2] Redoxâ€Neutral Cycloaddition of Nitrocyclopropanes with Styrenes by Visibleâ€Light Photocatalysis. Chemistry - A European Journal, 2015, 21, 9676-9680. | 1.7 | 37 |
| 21 | Directing-Group-Enabled Cycloaddition of Azides and Alkynes toward Functionalized Triazoles. Organic Letters, 2020, 22, 2220-2224. | 2.4 | 37 |
| 22 | Novel Guanidinium-Based Ionic Liquids for Highly Efficient SO<sub>2</sub> Capture. Journal of Physical Chemistry B, 2015, 119, 8054-8062. | 1.2 | 35 |
| 23 | Fabrication of lysozyme/Î²-carrageenan complex nanoparticles as a novel carrier to enhance the stability and in vitro release of curcumin. International Journal of Biological Macromolecules, 2020, 146, 444-452. | 3.6 | 35 |
| 24 | Intermolecular interactions between gold clusters and selected amino acids cysteine and glycine: a DFT study. Journal of Molecular Modeling, 2012, 18, 645-652. | 0.8 | 34 |
| 25 | DFT Studies on the Palladium-Catalyzed Dearomatization Reaction between Chloromethylnaphthalene and the Cyclic Amine Morpholine. Organometallics, 2013, 32, 2336-2343. | 1.1 | 33 |
| 26 | Encapsulation of curcumin in ZEIN-HTCC complexes: Physicochemical characterization, in vitro sustained release behavior and encapsulation mechanism. LWT - Food Science and Technology, 2022, 155, 112909. | 2.5 | 33 |
| 27 | Mechanisms and Reactivity Differences for Cycloaddition of Anhydride to Alkyne Catalyzed by Palladium and Nickel Catalysts: Insight from Density Functional Calculations. Journal of Organic Chemistry, 2014, 79, 11911-11921. | 1.7 | 32 |
| 28 | Enhanced in Vitro Antioxidant Activity of Polysaccharides From Enteromorpha Prolifera by Enzymatic Degradation. Journal of Food Biochemistry, 2016, 40, 275-283. | 1.2 | 31 |
| 29 | Stereocomplementary Chemoenzymatic Pictetâ€“Spengler Reactions for Formation of Rare Azepino-indole Frameworks: Discovery of Antimalarial Compounds. ACS Catalysis, 2019, 9, 7443-7448. | 5.5 | 31 |
| 30 | Isolation and absolute configurations of diastereomers of 8Î±-hydroxy-T-muurolol and (1Î±,6Î²,7Î²)-cadinane-4-en-8Î±,10Î±-diol from Chimonanthus salicifolius. Phytochemistry, 2016, 122, 294-300. | 1.4 | 30 |
| 31 | The fabrication of novel zein and resveratrol covalent conjugates: Enhanced thermal stability, emulsifying and antioxidant properties. Food Chemistry, 2022, 374, 131612. | 4.2 | 30 |
| 32 | Combined Quantum Mechanics/Molecular Mechanics Study on the Reversible Isomerization of Glucose and Fructose Catalyzed by Pyrococcus furiosus Phosphoglucose Isomerase. Journal of the American Chemical Society, 2008, 130, 7022-7031. | 6.6 | 29 |
| 33 | Edible Antimicrobial Coating Incorporating a Polymeric Iron Chelator and Its Application in the Preservation of Surimi Product. Food and Bioprocess Technology, 2016, 9, 1031-1039. | 2.6 | 29 |
| 34 | Divergent Total Syntheses of (â^')-Crinipellins Facilitated by a HAT-Initiated Dowdâ€“Beckwith Rearrangement. Journal of the American Chemical Society, 2022, 144, 2495-2500. | 6.6 | 29 |
| 35 | Exploring the Interstitial Atom in the FeMo Cofactor of Nitrogenase: Insights from QM and QM/MM Calculations. Journal of Physical Chemistry B, 2008, 112, 11435-11439. | 1.2 | 28 |
| 36 | Nitric Oxide Adsorption and Reduction Reaction Mechanism on the Rh<sub>7</sub><sup>+</sup> Cluster: A Density Functional Theory Study. Journal of Physical Chemistry A, 2011, 115, 14203-14208. | 1.1 | 28 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Understanding the Reactivity Difference of Isocyanate and Isothiocyanate toward a Ruthenium Silylene Hydride Complex. Organometallics, 2014, 33, 892-897. | 1.1 | 28 |
| 38 | Nanoengineered on-demand drug delivery system improves efficacy of pharmacotherapy for epilepsy. Science Advances, 2022, 8, eabm3381. | 4.7 | 27 |
| 39 | Volumetric property of glycine, l-serine, l-alanine and l-proline in aqueous solutions of 1-phenylpiperazinium tetrafluoroborate. Journal of Chemical Thermodynamics, 2016, 99, 75-81. | 1.0 | 26 |
| 40 | Skeletal reorganization divergence of N-sulfonyl ynamides. Nature Communications, 2020, 11, 5639. | 5.8 | 26 |
| 41 | New progress in theoretical studies on palladium-catalyzed Câ˜C bond-forming reaction mechanisms. Science China Chemistry, 2016, 59, 1432-1447. | 4.2 | 24 |
| 42 | A DFT Study on Palladium and Nickel-Catalyzed Regioselective and Stereoselective Hydrosilylation of 1,3-Disubstituted Allenes. Organometallics, 2017, 36, 3371-3381. | 1.1 | 24 |
| 43 | Real-Time In Situ Screening of Omega-7 Phospholipids in Marine Biological Resources Using an iKnife-Rapid-Evaporative-Ionization-Mass-Spectrometry-Based Lipidomics Phenotype. Journal of Agricultural and Food Chemistry, 2021, 69, 9004-9011. | 2.4 | 24 |
| 44 | A divergent [5+2] cascade approach to bicyclo[3.2.1]octanes: facile synthesis of ent-kaurene and cedrene-type skeletons. Chemical Communications, 2017, 53, 8435-8438. | 2.2 | 23 |
| 45 | Densities and viscosities of binary mixtures of 2,2-diethyl-1,1,3,3-tetramethylguanidinium bis(trifluoromethylsulfonyl)imide with methanol and ethanol. Journal of Chemical Thermodynamics, 2019, 136, 44-53. | 1.0 | 23 |
| 46 | Structural transitions of ovalbumin/Î¹-carrageenan complexes under the effects of pH and composition. Chemical Physics, 2020, 533, 110733. | 0.9 | 23 |
| 47 | Thermal Decomposition Kinetics and Mechanism of 1,1â€²-Bicyclohexyl. Energy & Fuels, 2014, 28, 4523-4531. | 2.5 | 22 |
| 48 | A chelating polymer resin: synthesis, characterization, adsorption and desorption performance for removal of Hg(II) from aqueous solution. Journal of the Iranian Chemical Society, 2017, 14, 2557-2566. | 1.2 | 22 |
| 49 | Triazenyl Alkynes as Versatile Building Blocks in Multicomponent Reactions: Diastereoselective Synthesis of Î²â€Amino Amides. Angewandte Chemie - International Edition, 2021, 60, 5147-5151. | 7.2 | 22 |
| 50 | Mechanism and Substrate-Dependent Rate-Determining Step in Palladium-Catalyzed Intramolecular Decarboxylative Coupling of Arenecarboxylic Acids with Aryl Bromides: A DFT Study. Organometallics, 2013, 32, 6957-6968. | 1.1 | 21 |
| 51 | DFT studies on the mechanisms of palladium-catalyzed intramolecular arylation of a silyl C(sp3)â€“H bond. New Journal of Chemistry, 2013, 37, 2856. | 1.4 | 20 |
| 52 | Solute-solvent interactions of amino acid l -phenylalanine in aqueous 1-butyl-2,3-dimethylimidazolium bromide ionic liquid solutions. Journal of Chemical Thermodynamics, 2017, 113, 144-150. | 1.0 | 20 |
| 53 | Investigations on the thermal decomposition of JP-10/ iso -octane binary mixtures. Fuel, 2016, 163, 148-156. | 3.4 | 19 |
| 54 | Influence of Molecular Structure on Contact Interaction between Thiophene Anchoring Group and Au Electrode. Journal of Physical Chemistry C, 2017, 121, 1472-1476. | 1.5 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Enzymatic Reduction of Nitrate to Nitrite: Insight from Density Functional Calculations. Organometallics, 2010, 29, 436-441. | 1.1 | 18 |
| 56 | Fabrication of PGFE/CN-stabilized Î²-carotene-loaded peppermint oil nanoemulsions: Storage stability, rheological behavior and intelligent sensory analyses. LWT - Food Science and Technology, 2021, 138, 110688. | 2.5 | 18 |
| 57 | Enantioselective Total Synthesis of (+)â€Steenkrotinâ€...A and Determination of Its Absolute Configuration. Chemistry - A European Journal, 2016, 22, 959-970. | 1.7 | 17 |
| 58 | Quantitative proteomics reveals the relationship between protein changes and off-flavor in Russian sturgeon (Acipenser gueldenstaedti) fillets treated with low temperature vacuum heating. Food Chemistry, 2022, 370, 131371. | 4.2 | 17 |
| 59 | Theoretical and experimental perspectives of interaction mechanism between zein and lysozyme. Food Hydrocolloids, 2022, 132, 107876. | 5.6 | 17 |
| 60 | Phase behaviors and curcumin encapsulation performance of Gemini surfactant microemulsion. Journal of Molecular Liquids, 2020, 315, 113786. | 2.3 | 16 |
| 61 | Exploration of the Microstructure and Rheological Properties of Sodium Alginate-Pectin-Whey Protein Isolate Stabilized Î²-Carotene Emulsions: To Improve Stability and Achieve Gastrointestinal Sustained Release. Foods, 2021, 10, 1991. | 1.9 | 16 |
| 62 | Recent advances in theoretical studies on ligand-controlled selectivity of nickel- and palladium-catalyzed cross-coupling reactions. Chinese Chemical Letters, 2021, 32, 319-327. | 4.8 | 15 |
| 63 | A polyester-based initiation strategy for achieving high-efficient cracking of hydrocarbon fuels. Chemical Engineering Journal, 2021, 425, 128059. | 6.6 | 15 |
| 64 | Asymmetric Total Syntheses of (+)-Davisinol and (+)-18-Benzoyldavisinol: A HAT-Initiated Transannular Redox Radical Approach. Journal of the American Chemical Society, 2021, 143, 10576-10581. | 6.6 | 15 |
| 65 | Structureâ€“Function Analysis of the Conserved Tyrosine and Diverse Ï€-Stacking among Class I Histone Deacetylases: A QM (DFT)/MM MD Study. Journal of Chemical Information and Modeling, 2014, 54, 3162-3171. | 2.5 | 14 |
| 66 | Palladium(0)-Catalyzed Methylcyclopropanation of Norbornenes with Vinyl Bromides and Mechanism Study. Organic Letters, 2015, 17, 3678-3681. | 2.4 | 14 |
| 67 | Why different ligands can control stereochemistry selectivity of Ni-catalyzed Suzukiâ€“Miyaura cross-coupling of benzylic carbamates with arylboronic esters: a mechanistic study. Dalton Transactions, 2017, 46, 13010-13019. | 1.6 | 14 |
| 68 | Substrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity. ACS Catalysis, 2017, 7, 5841-5846. | 5.5 | 14 |
| 69 | Strategically designed macromolecules as additives for high energy-density hydrocarbon fuels. Fuel, 2020, 270, 117433. | 3.4 | 14 |
| 70 | Insight into the effect of ultrasound treatment on the rheological properties of myofibrillar proteins based on the changes in their tertiary structure. Food Research International, 2022, 157, 111136. | 2.9 | 14 |
| 71 | Explore the Catalytic Reaction Mechanism in the Reduction of NO by CO on the Rh<sub>7</sub><sup>+</sup> Cluster: A Quantum Chemical Study. Journal of Physical Chemistry C, 2012, 116, 7776-7781. | 1.5 | 13 |
| 72 | A quantum chemistry study on thermochemical properties of high energy-density endothermic hydrocarbon fuel JP-10. Journal of Molecular Modeling, 2014, 20, 2183. | 0.8 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Isolation and lipidomics characterization of fatty acids and phospholipids in shrimp waste through GC/FID and HILIC-QTrap/MS. Journal of Food Composition and Analysis, 2021, 95, 103668. | 1.9 | 13 |
| 74 | Preparation of zein-lecithin-EGCG complex nanoparticles stabilized peppermint oil emulsions: Physicochemical properties, stability and intelligent sensory analysis. Food Chemistry, 2022, 383, 132453. | 4.2 | 13 |
| 75 | Effects of electron attachment on C<sub>5â€²</sub>ï£¿O<sub>5â€²</sub> and C<sub>1â€²</sub>ï£¿N<sub>1</sub> bond cleavages of pyrimidine nucleotides: A theoretical study. Journal of Computational Chemistry, 2008, 29, 2025-2032. | 1.5 | 12 |
| 76 | Radical Scavenging Activity of Myricetin. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 1421-1432. | 2.2 | 12 |
| 77 | Mechanistic insights into small molecule activation induced by ligand cooperativity in PCcarbeneP nickel pincer complexes: a quantum chemistry study. Journal of Molecular Modeling, 2015, 21, 242. | 0.8 | 12 |
| 78 | Quantum interference effect of single-molecule conductance influenced by insertion of different alkyl length. Electrochemistry Communications, 2016, 68, 86-89. | 2.3 | 12 |
| 79 | Modified Hyperbranched Polyglycerol as Dispersant for Size Control and Stabilization of Gold Nanoparticles in Hydrocarbons. Nanoscale Research Letters, 2017, 12, 525. | 3.1 | 12 |
| 80 | Low Tunneling Decay of Iodine-Terminated Alkane Single-Molecule Junctions. Nanoscale Research Letters, 2018, 13, 121. | 3.1 | 12 |
| 81 | Fabrication and characterization of oil-in-water pickering emulsions stabilized by ZEIN-HTCC nanoparticles as a composite layer. Food Research International, 2021, 148, 110606. | 2.9 | 12 |
| 82 | Electron attachment to the DNA bases adenine and guanine and dehydrogenation of their anionic derivatives: Density functional study. International Journal of Quantum Chemistry, 2007, 107, 1261-1269. | 1.0 | 11 |
| 83 | Density functional study of protonation of deoxynucleosides: Electrophilic active sites and proton affinities. International Journal of Quantum Chemistry, 2008, 108, 57-65. | 1.0 | 11 |
| 84 | A DFT study on the thermal cracking of JP-10. Journal of Molecular Modeling, 2013, 19, 5355-5365. | 0.8 | 11 |
| 85 | A DFT study on palladium-catalyzed decarboxylative intramolecular aziridination reaction mechanism. Journal of Organometallic Chemistry, 2013, 745-746, 417-422. | 0.8 | 11 |
| 86 | Conformational Isomerism Influence on the Properties of Piperazinium Bis(trifluoromethylsulfonyl)imide. Journal of Physical Chemistry B, 2014, 118, 9085-9095. | 1.2 | 11 |
| 87 | Explore the reaction mechanism of the Maillard reaction: a density functional theory study. Journal of Molecular Modeling, 2015, 21, 132. | 0.8 | 11 |
| 88 | A DFT study on the mechanisms of hydrogenation and hydrosilylation of nitrous oxide catalyzed by a ruthenium PNP pincer complex. Computational and Theoretical Chemistry, 2018, 1128, 48-55. | 1.1 | 11 |
| 89 | Total Synthesis of (+)-Jatrophalactam. Organic Letters, 2019, 21, 9603-9607. | 2.4 | 11 |
| 90 | Pyrolysis kinetics and mechanism of ethylcyclohexane. Journal of Analytical and Applied Pyrolysis, 2020, 145, 104723. | 2.6 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Green Extraction of Phenolic Compounds from Lotus Seedpod (Receptaculum Nelumbinis) Assisted by Ultrasound Coupled with Glycerol. Foods, 2021, 10, 239. | 1.9 | 11 |
| 92 | Distribution of pigments in the aqueous two-phase system formed with piperazinium-based ionic liquid and anionic surfactant. Journal of Molecular Liquids, 2021, 330, 115677. | 2.3 | 11 |
| 93 | An AIL/IL-based liquid/liquid extraction system for the purification of His-tagged proteins. Applied Microbiology and Biotechnology, 2014, 98, 5665-5675. | 1.7 | 10 |
| 94 | Dehydrogenation of benzyl alcohol with N<sub>2</sub>O as the hydrogen acceptor catalyzed by the rhodium(<scp>i</scp>) carbene complex: insights from quantum chemistry calculations. Dalton Transactions, 2016, 45, 16485-16491. | 1.6 | 10 |
| 95 | DFT studies on mechanistic origins of ligand-controlled selectivity in Pd-catalyzed non-decarbonylative and decarbonylative reductive conversion of acyl fluoride. Dalton Transactions, 2019, 48, 3440-3446. | 1.6 | 10 |
| 96 | Low-salted salmon: Effects of salt reduction on physicochemical, lipidomic, and sensory characteristics. LWT - Food Science and Technology, 2021, 152, 112311. | 2.5 | 10 |
| 97 | One-Step Cyclization: Synthesis of N-Heteroalkyl-Nâ€²-tosylpiperazines. Journal of Organic Chemistry, 2012, 77, 7506-7511. | 1.7 | 9 |
| 98 | Reaction Mechanisms of a Tungstenâ€“Germylyne Complex with One or Two Molecules of Alcohols and Arylaldehydes: A DFT Study. European Journal of Inorganic Chemistry, 2014, 2014, 1502-1511. | 1.0 | 9 |
| 99 | Density Functional Study toward Understanding Dehydrogenation of the Adenineâ‹¯Thymine Base Pair and Its Anion. Journal of Physical Chemistry A, 2007, 111, 4384-4390. | 1.1 | 8 |
| 100 | Broad Substrate Specificity and Catalytic Mechanism of Pseudomonas stutzeri <scp>l</scp>-Rhamnose Isomerase: Insights from QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 11595-11603. | 1.1 | 8 |
| 101 | Theoretical studies on the reductive elimination reaction mechanism from neutral palladium(IV) sulfinate complexes. Journal of Physical Organic Chemistry, 2013, 26, 933-938. | 0.9 | 8 |
| 102 | Formation of Novel Aqueous Two-Phase Systems with Piperazinium-Based Ionic Liquids and Anionic Surfactants: Phase Behavior and Microstructure. Journal of Physical Chemistry B, 2015, 119, 11798-11806. | 1.2 | 8 |
| 103 | Electrostatic-driven structural transformation in the complexation of lysozyme and Î°-carrageenan. Chemical Physics, 2020, 538, 110910. | 0.9 | 8 |
| 104 | Mechanism of Carbon Monoxide Induced Nâ€“N Bond Cleavage of Nitrous Oxide Mediated by Molybdenum Complexes: A DFT Study. Organometallics, 2014, 33, 1553-1562. | 1.1 | 7 |
| 105 | The mechanisms for triple gold(I)-catalyzed (4+1) cycloaddition of methylenecyclopropane with 7-naphthyl-1,3,5-cycloheptatriene: Insight into from density functional calculations. Computational and Theoretical Chemistry, 2016, 1084, 25-35. | 1.1 | 7 |
| 106 | Protein-peptide nutritional material prepared from surimi wash-water using immobilized chymotrypsin-trypsin. Journal of the Science of Food and Agriculture, 2017, 97, 1746-1752. | 1.7 | 7 |
| 107 | Side-Group Effect on Electron Transport of Single Molecular Junctions. Micromachines, 2018, 9, 234. | 1.4 | 7 |
| 108 | Oxidation of phenyl and hydride ligands of bis(pentamethylcyclopentadienyl)hafnium derivatives by nitrous oxide via selective oxygen atom transfer reactions: insights from quantum chemistry calculations. Dalton Transactions, 2016, 45, 1152-1159. | 1.6 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Non-innocent PNN ligand is important for CO oxidation by N<sub>2</sub>O catalyzed by a (PNN)Ruâ€“H pincer complex: insights from DFT calculations. Dalton Transactions, 2018, 47, 15324-15330. | 1.6 | 6 |
| 110 | Key Mechanistic Features in Palladium-Catalyzed Methylcyclopropanation of Norbornenes With Vinyl Bromides: Insights From DFT Calculations. Frontiers in Chemistry, 2019, 7, 169. | 1.8 | 6 |
| 111 | Phospholipidomics quality evaluation of swimming crabs (Portunus trituberculatus) cultured with formulated feed, frozen trash fish, and mixed feed, a non-target approach by HILIC-MS. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2021, 1179, 122845. | 1.2 | 6 |
| 112 | Oxygenolysis reaction mechanism of copper-dependent quercetin 2,3-dioxygenase: A density functional theory study. Science China Chemistry, 2012, 55, 1832-1841. | 4.2 | 5 |
| 113 | Mechanisms of chemoselectivity for acyl and decarbonylative Suzukiâ€“Miyaura coupling of N-acetyl amide with arylboronic acid catalyzed by Pd and Ni catalysts: Insights from DFT calculations. Computational and Theoretical Chemistry, 2020, 1185, 112889. | 1.1 | 5 |
| 114 | Characterization of Metabolites in a Zebrafish Model of Alzheimerâ€™s Disease Supplemented with Mussel-Derived Plasmalogens by Ultraperformance Liquid Chromatography Q-Exactive Orbitrap Mass Spectrometry-Based Unbiased Metabolomics. Journal of Agricultural and Food Chemistry, 2021, 69, 12187-12196. | 2.4 | 5 |
| 115 | Insights into the enzymatic catalytic mechanism of bCinS: the importance of protein conformational change. Catalysis Science and Technology, 2022, 12, 1651-1662. | 2.1 | 5 |
| 116 | Exploring the reaction mechanism of a cationic terminal iridium methylene complex with ethyl diazoacetate, a Lewis base and dihydrogen: a quantum chemistry study. New Journal of Chemistry, 2014, 38, 4115. | 1.4 | 4 |
| 117 | The Interactions between Quaternary Ammonium Cationic Surfactants and Bovine Serum Albumin. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 2951-2960. | 2.2 | 4 |
| 118 | The reactivity of coordinatively unsaturated iridium methylene complex Ir CH2[N(SiMe2CH2PPh2)2]: A quantum chemistry study. Computational and Theoretical Chemistry, 2018, 1138, 91-98. | 1.1 | 4 |
| 119 | Catalytic Coupling of CH<sub>4</sub> with CO<sub>2</sub> and CO by a Modified Human Carbonic Anhydrase Combined with Oriented External Electric Fields: Mechanistic Insights from DFT Calculations. Organometallics, 2020, 39, 4657-4666. | 1.1 | 4 |
| 120 | Iridium(<scp>i</scp>)-catalyzed hydration/esterification of 2-alkynylphenols and carboxylic acids. Chemical Communications, 2020, 56, 3093-3096. | 2.2 | 4 |
| 121 | Characterization and stability of peppermint oil emulsions using polyglycerol esters of fatty acids and milk proteins as emulsifiers. Journal of Food Science, 2021, 86, 5148-5158. | 1.5 | 4 |
| 122 | Pdâ€catalyzed bicyclization of 2â€alkynylhalobenzenes and propargylic alcohols for the formation of indeno[1,2]furans: a DFT study. Journal of Physical Organic Chemistry, 2014, 27, 237-244. | 0.9 | 3 |
| 123 | Theoretically exploring the key role of the Lys412 residue in the conversion of N<sub>2</sub>O to N<sub>2</sub>by nitrous oxide reductase from Achromobacter cycloclastes. New Journal of Chemistry, 2015, 39, 8093-8099. | 1.4 | 3 |
| 124 | Microstructures of the Gemini surfactant microemulsion system 14-4-14/1-propanol/n-heptane/water. Journal of Molecular Liquids, 2020, 320, 114485. | 2.3 | 3 |
| 125 | Complexation of Î²â€lactoglobulin with gum arabic: Effect of heat treatment and enhanced encapsulation efficiency. Food Science and Nutrition, 2021, 9, 1399-1409. | 1.5 | 3 |
| 126 | Mechanistic study on oxidative degradation and deposition of exo-tetrahydrodicyclopentadiene. Fuel, 2022, 317, 123533. | 3.4 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Understanding hydrogenation of the adenineâ€¢thymine base pairs and their anions: A density functional study. International Journal of Quantum Chemistry, 2012, 112, 609-618. | 1.0 | 2 |
| 128 | Translocation of a Polymer through a Crowded Channel under Electrical Force. BioMed Research International, 2017, 2017, 1-7. | 0.9 | 2 |
| 129 | Reply to Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€• ACS Catalysis, 2018, 8, 1363-1370. | 5.5 | 2 |
| 130 | A combined experimental and theoretical study on the structures, interactions and volumetric properties of guanidinium-based ionic liquid mixtures. Physical Chemistry Chemical Physics, 2019, 21, 17720-17728. | 1.3 | 2 |
| 131 | A DFT study on the mechanism and origins of the ligand-controlled regioselectivity of a palladium-catalyzed dearomatic reaction of 1-(chloromethyl)naphthalene with phenylacetonitrile. New Journal of Chemistry, 2019, 43, 19120-19125. | 1.4 | 2 |
| 132 | Triazenyl Alkynes as Versatile Building Blocks in Multicomponent Reactions: Diastereoselective Synthesis of Î²â€Amino Amides. Angewandte Chemie, 2021, 133, 5207-5211. | 1.6 | 2 |
| 133 | Lipidomics study on the molecular changes of eicosapentaenoic and docosahexaenoic acyl structured glycerides during enzyme-catalysis and chemocatalysis. LWT - Food Science and Technology, 2021, 148, 111815. | 2.5 | 2 |
| 134 | Investigation of interfacial composition and thermodynamic stability of 14-n-14/alcohol/oil/water microemulsions by dilution method. Journal of Molecular Liquids, 2021, 336, 116333. | 2.3 | 2 |
| 135 | N-Insertion reaction mechanisms of phenyl azides with a hafnium hydride complex: a quantum chemistry calculation. New Journal of Chemistry, 2017, 41, 5007-5011. | 1.4 | 1 |
| 136 | A substrate-dependent mechanism for the reactions of a hydrido(hydrosilylene)ruthenium complex with carbonyl compounds: insights from quantum chemical calculations. New Journal of Chemistry, 2017, 41, 198-203. | 1.4 | 1 |
| 137 | Tuning the conformations of hemoglobin via interactions with single-chain and Gemini quaternary ammonium surfactants. Chemical Physics Letters, 2019, 728, 115-123. | 1.2 | 1 |
| 138 | Mechanism in palladium-catalyzed dearomative allylic reactions of benzyl phosphates with allyl borates: Insights from DFT calculations. Computational and Theoretical Chemistry, 2020, 1191, 113030. | 1.1 | 1 |
| 139 | Reaction Mechanism for the Alkoxylation of a Silyl Ligand in the Silyl- (silylene)ruthenium Complex: A Density Functional Theory Study. Chinese Journal of Organic Chemistry, 2015, 35, 698. | 0.6 | 0 |