

Hujun Xie

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

137
papers

1,847
citations

24
h-index

34
g-index

146
ext. papers

2,469
ext. citations

5.7
avg, IF

5.31
L-index

#	Paper	IF	Citations
137	Nanoengineered on-demand drug delivery system improves efficacy of pharmacotherapy for epilepsy.. <i>Science Advances</i> , 2022 , 8, eabm3381	14.3	4
136	Divergent Total Syntheses of (-)-Crinipellins Facilitated by a HAT-Initiated Dowd-Beckwith Rearrangement.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	4
135	Preparation of zein-lecithin-EGCG complex nanoparticles stabilized peppermint oil emulsions: Physicochemical properties, stability and intelligent sensory analysis.. <i>Food Chemistry</i> , 2022 , 383, 132453	8.5	0
134	Quantitative proteomics reveals the relationship between protein changes and off-flavor in Russian sturgeon (<i>Acipenser gueldenstaedti</i>) fillets treated with low temperature vacuum heating. <i>Food Chemistry</i> , 2022 , 370, 131371	8.5	2
133	Mechanistic study on oxidative degradation and deposition of exo-tetrahydrodicyclopentadiene. <i>Fuel</i> , 2022 , 317, 123533	7.1	0
132	Insight into the effect of ultrasound treatment on the rheological properties of myofibrillar proteins based on the changes in their tertiary structure. <i>Food Research International</i> , 2022 , 157, 111136	7	1
131	The fabrication of novel zein and resveratrol covalent conjugates: Enhanced thermal stability, emulsifying and antioxidant properties. <i>Food Chemistry</i> , 2021 , 374, 131612	8.5	1
130	Characterization and stability of peppermint oil emulsions using polyglycerol esters of fatty acids and milk proteins as emulsifiers. <i>Journal of Food Science</i> , 2021 , 86, 5148	3.4	1
129	Encapsulation of curcumin in ZEIN-HTCC complexes: Physicochemical characterization, in vitro sustained release behavior and encapsulation mechanism. <i>LWT - Food Science and Technology</i> , 2021 , 155, 112909	5.4	2
128	Characterization of Metabolites in a Zebrafish Model of Alzheimer's Disease Supplemented with Mussel-Derived Plasmalogens by Ultraperformance Liquid Chromatography Q-Exactive Orbitrap Mass Spectrometry-Based Unbiased Metabolomics. <i>Journal of Agricultural and Food Chemistry</i> , 2021 69, 12187-12195	5.7	0
127	Fabrication of PGFE/CN-stabilized β -carotene-loaded peppermint oil nanoemulsions: Storage stability, rheological behavior and intelligent sensory analyses. <i>LWT - Food Science and Technology</i> , 2021 , 138, 110688	5.4	6
126	Development of antifungal gelatin-based nanocomposite films functionalized with natamycin-loaded zein/casein nanoparticles. <i>Food Hydrocolloids</i> , 2021 , 113, 106506	10.6	29
125	Distribution of pigments in the aqueous two-phase system formed with piperazinium-based ionic liquid and anionic surfactant. <i>Journal of Molecular Liquids</i> , 2021 , 330, 115677	6	0
124	Application of whey protein isolate fibrils in encapsulation and protection of β -carotene. <i>Food Chemistry</i> , 2021 , 346, 128963	8.5	11
123	Recent advances in theoretical studies on ligand-controlled selectivity of nickel- and palladium-catalyzed cross-coupling reactions. <i>Chinese Chemical Letters</i> , 2021 , 32, 319-327	8.1	4
122	Isolation and lipidomics characterization of fatty acids and phospholipids in shrimp waste through GC/FID and HILIC-QTrap/MS. <i>Journal of Food Composition and Analysis</i> , 2021 , 95, 103668	4.1	6
121	A polyester-based initiation strategy for achieving high-efficient cracking of hydrocarbon fuels. <i>Chemical Engineering Journal</i> , 2021 , 425, 128059	14.7	4

120	The regulation of sodium alginate on the stability of ovalbumin-pectin complexes for VD encapsulation and in vitro simulated gastrointestinal digestion study. <i>Food Research International</i> , 2021 , 140, 110011	7	16
119	Triazenyl Alkynes as Versatile Building Blocks in Multicomponent Reactions: Diastereoselective Synthesis of β -Amino Amides. <i>Angewandte Chemie</i> , 2021 , 133, 5207-5211	3.6	
118	Triazenyl Alkynes as Versatile Building Blocks in Multicomponent Reactions: Diastereoselective Synthesis of β -Amino Amides. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 5147-5151	16.4	10
117	Complexation of β -lactoglobulin with gum arabic: Effect of heat treatment and enhanced encapsulation efficiency. <i>Food Science and Nutrition</i> , 2021 , 9, 1399-1409	3.2	1
116	Green Extraction of Phenolic Compounds from Lotus Seedpod () Assisted by Ultrasound Coupled with Glycerol. <i>Foods</i> , 2021 , 10,	4.9	6
115	Asymmetric Total Syntheses of (+)-Davisinol and (+)-18-Benzoyldavisinol: A HAT-Initiated Transannular Redox Radical Approach. <i>Journal of the American Chemical Society</i> , 2021 , 143, 10576-10581	16.4	4
114	Lipidomics study on the molecular changes of eicosapentaenoic and docosahexaenoic acyl structured glycerides during enzyme-catalysis and chemocatalysis. <i>LWT - Food Science and Technology</i> , 2021 , 148, 111815	5.4	0
113	Preparation of β -lactoglobulin/gum arabic complex nanoparticles for encapsulation and controlled release of EGCG in simulated gastrointestinal digestion model. <i>Food Chemistry</i> , 2021 , 354, 129516	8.5	18
112	Phospholipidomics quality evaluation of swimming crabs (<i>Portunus trituberculatus</i>) cultured with formulated feed, frozen trash fish, and mixed feed, a non-target approach by HILIC-MS. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2021 , 1179, 122845	3.2	2
111	Investigation of interfacial composition and thermodynamic stability of 14-n-14/alcohol/oil/water microemulsions by dilution method. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116333	6	1
110	Curcumin-loaded core-shell biopolymer nanoparticles produced by the pH-driven method: Physicochemical and release properties. <i>Food Chemistry</i> , 2021 , 355, 129686	8.5	23
109	Fabrication and characterization of oil-in-water pickering emulsions stabilized by ZEIN-HTCC nanoparticles as a composite layer. <i>Food Research International</i> , 2021 , 148, 110606	7	3
108	Explore the interaction mechanism between zein and EGCG using multi-spectroscopy and molecular dynamics simulation methods. <i>Food Hydrocolloids</i> , 2021 , 120, 106906	10.6	19
107	Fabrication of Zein-Lecithin-EGCG complex nanoparticles: Characterization, controlled release in simulated gastrointestinal digestion. <i>Food Chemistry</i> , 2021 , 365, 130542	8.5	9
106	Low-salted salmon: Effects of salt reduction on physicochemical, lipidomic, and sensory characteristics. <i>LWT - Food Science and Technology</i> , 2021 , 152, 112311	5.4	1
105	Real-Time Screening of Omega-7 Phospholipids in Marine Biological Resources Using an iKnife-Rapid-Evaporative-Ionization-Mass-Spectrometry-Based Lipidomics Phenotype. <i>Journal of Agricultural and Food Chemistry</i> , 2021 , 69, 9004-9011	5.7	14
104	Catalytic Coupling of CH ₄ with CO ₂ and CO by a Modified Human Carbonic Anhydrase Combined with Oriented External Electric Fields: Mechanistic Insights from DFT Calculations. <i>Organometallics</i> , 2020 , 39, 4657-4666	3.8	3
103	Mechanisms of chemoselectivity for acyl and decarbonylative SuzukiMiyaura coupling of N-acetyl amide with arylboronic acid catalyzed by Pd and Ni catalysts: Insights from DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2020 , 1185, 112889	2	2

102	Highly transparent, self-healing conductive elastomers enabled by synergistic hydrogen bonding interactions. <i>Chemical Engineering Journal</i> , 2020 , 393, 124685	14.7	39
101	Strategically designed macromolecules as additives for high energy-density hydrocarbon fuels. <i>Fuel</i> , 2020 , 270, 117433	7.1	10
100	Directing-Group-Enabled Cycloaddition of Azides and Alkynes toward Functionalized Triazoles. <i>Organic Letters</i> , 2020 , 22, 2220-2224	6.2	25
99	Electrostatic-driven structural transformation in the complexation of lysozyme and κ -carrageenan. <i>Chemical Physics</i> , 2020 , 538, 110910	2.3	0
98	Structural transitions of ovalbumin/ κ -carrageenan complexes under the effects of pH and composition. <i>Chemical Physics</i> , 2020 , 533, 110733	2.3	10
97	Fabrication of lysozyme/ κ -carrageenan complex nanoparticles as a novel carrier to enhance the stability and in vitro release of curcumin. <i>International Journal of Biological Macromolecules</i> , 2020 , 146, 444-452	7.9	16
96	Iridium(i)-catalyzed hydration/esterification of 2-alkynylphenols and carboxylic acids. <i>Chemical Communications</i> , 2020 , 56, 3093-3096	5.8	4
95	Development of ovalbumin-pectin nanocomplexes for vitamin D3 encapsulation: Enhanced storage stability and sustained release in simulated gastrointestinal digestion. <i>Food Hydrocolloids</i> , 2020 , 106, 105926	10.6	46
94	Pyrolysis kinetics and mechanism of ethylcyclohexane. <i>Journal of Analytical and Applied Pyrolysis</i> , 2020 , 145, 104723	6	4
93	Mechanism in palladium-catalyzed dearomative allylic reactions of benzyl phosphates with allyl borates: Insights from DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2020 , 1191, 113030	2	1
92	Phase behaviors and curcumin encapsulation performance of Gemini surfactant microemulsion. <i>Journal of Molecular Liquids</i> , 2020 , 315, 113786	6	8
91	Skeletal reorganization divergence of N-sulfonyl ynarnides. <i>Nature Communications</i> , 2020 , 11, 5639	17.4	10
90	Microstructures of the Gemini surfactant microemulsion system 14-4-14/1-propanol/n-heptane/water. <i>Journal of Molecular Liquids</i> , 2020 , 320, 114485	6	2
89	Chameleon-like Behavior of the Directing Group in the Rh(III)-Catalyzed Regioselective C-H Amidation of Indole: An Experimental and Computational Study. <i>ACS Catalysis</i> , 2019 , 9, 10233-10244	13.1	27
88	Tuning the conformations of hemoglobin via interactions with single-chain and Gemini quaternary ammonium surfactants. <i>Chemical Physics Letters</i> , 2019 , 728, 115-123	2.5	0
87	Densities and viscosities of binary mixtures of 2,2-diethyl-1,1,3,3-tetramethylguanidinium bis(trifluoromethylsulfonyl)imide with methanol and ethanol. <i>Journal of Chemical Thermodynamics</i> , 2019 , 136, 44-53	2.9	16
86	Controllable hierarchical self-assembly of porphyrin-derived supra-amphiphiles. <i>Nature Communications</i> , 2019 , 10, 1399	17.4	28
85	Key Mechanistic Features in Palladium-Catalyzed Methylcyclopropanation of Norbornenes With Vinyl Bromides: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019 , 7, 169	5	3

84	DFT studies on mechanistic origins of ligand-controlled selectivity in Pd-catalyzed non-decarbonylative and decarbonylative reductive conversion of acyl fluoride. <i>Dalton Transactions</i> , 2019 , 48, 3440-3446	4.3	7
83	Stereocomplementary Chemoenzymatic Pictet-Spengler Reactions for Formation of Rare Azepino-indole Frameworks: Discovery of Antimalarial Compounds. <i>ACS Catalysis</i> , 2019 , 9, 7443-7448	13.1	22
82	A combined experimental and theoretical study on the structures, interactions and volumetric properties of guanidinium-based ionic liquid mixtures. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 17720-17728	3.6	1
81	Total Synthesis of (+)-Jatropha lactam. <i>Organic Letters</i> , 2019 , 21, 9603-9607	6.2	8
80	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. <i>New Journal of Chemistry</i> , 2019 , 43, 19120-19125	3.6	2
79	Fabrication of ovalbumin/κ-carrageenan complex nanoparticles as a novel carrier for curcumin delivery. <i>Food Hydrocolloids</i> , 2019 , 89, 111-121	10.6	78
78	A DFT study on the mechanisms of hydrogenation and hydrosilylation of nitrous oxide catalyzed by a ruthenium PNP pincer complex. <i>Computational and Theoretical Chemistry</i> , 2018 , 1128, 48-55	2	8
77	Reply to Comment on Substrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity. <i>ACS Catalysis</i> , 2018 , 8, 1363-1370	13.1	2
76	Side-Group Effect on Electron Transport of Single Molecular Junctions. <i>Micromachines</i> , 2018 , 9,	3.3	4
75	The reactivity of coordinatively unsaturated iridium methylene complex Ir CH ₂ [N(SiMe ₂ CH ₂ PPh ₂) ₂]: A quantum chemistry study. <i>Computational and Theoretical Chemistry</i> , 2018 , 1138, 91-98	2	4
74	Low Tunneling Decay of Iodine-Terminated Alkane Single-Molecule Junctions. <i>Nanoscale Research Letters</i> , 2018 , 13, 121	5	10
73	Iron-Catalyzed Enantioselective Si-H Bond Insertions. <i>Organic Letters</i> , 2018 , 20, 6544-6549	6.2	33
72	Non-innocent PNN ligand is important for CO oxidation by NO catalyzed by a (PNN)Ru-H pincer complex: insights from DFT calculations. <i>Dalton Transactions</i> , 2018 , 47, 15324-15330	4.3	4
71	Spirooxindole synthesis via palladium-catalyzed dearomatic reductive-Heck reaction. <i>Organic and Biomolecular Chemistry</i> , 2017 , 15, 2711-2715	3.9	47
70	N-Insertion reaction mechanisms of phenyl azides with a hafnium hydride complex: a quantum chemistry calculation. <i>New Journal of Chemistry</i> , 2017 , 41, 5007-5011	3.6	
69	Solute-solvent interactions of amino acid l-phenylalanine in aqueous 1-butyl-2,3-dimethylimidazolium bromide ionic liquid solutions. <i>Journal of Chemical Thermodynamics</i> , 2017 , 113, 144-150	2.9	14
68	Influence of Molecular Structure on Contact Interaction between Thiophene Anchoring Group and Au Electrode. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1472-1476	3.8	13
67	Modified Hyperbranched Polyglycerol as Dispersant for Size Control and Stabilization of Gold Nanoparticles in Hydrocarbons. <i>Nanoscale Research Letters</i> , 2017 , 12, 525	5	9

- 66 A DFT Study on Palladium and Nickel-Catalyzed Regioselective and Stereoselective Hydrosilylation of 1,3-Disubstituted Allenes. *Organometallics*, **2017**, 36, 3371-3381 3.8 21
- 65 Why different ligands can control stereochemistry selectivity of Ni-catalyzed Suzuki-Miyaura cross-coupling of benzylic carbamates with arylboronic esters: a mechanistic study. *Dalton Transactions*, **2017**, 46, 13010-13019 4.3 11
- 64 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 2 13
- 63 Substrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity. *ACS Catalysis*, **2017**, 7, 5841-5846 13.1 13
- 62 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 5.8 18
- 61 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 3.6 1
- 60 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 4.3 5
- 59 Translocation of a Polymer through a Crowded Channel under Electrical Force. *BioMed Research International*, **2017**, 2017, 5267185 3 1
- 58 New progress in theoretical studies on palladium-catalyzed C-C bond-forming reaction mechanisms. *Science China Chemistry*, **2016**, 59, 1432-1447 7.9 17
- 57 Visible-Light Promoted Distereodivergent Intramolecular Oxyamidation of Alkenes. *Chemistry - A European Journal*, **2016**, 22, 18695-18699 4.8 33
- 56 Enhanced in Vitro Antioxidant Activity of Polysaccharides From *Enteromorpha Prolifera* by Enzymatic Degradation. *Journal of Food Biochemistry*, **2016**, 40, 275-283 3.3 22
- 55 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 2 7
- 54 Isolation and absolute configurations of diastereomers of 8-hydroxy-T-muurolol and (1R,7R)-cadinane-4-en-8-ol diol from *Chimonanthus salicifolius*. *Phytochemistry*, **2016**, 122, 294-300 4 24
- 53 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 5.1 22
- 52 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, 1152-9 4.3 5
- 51 Investigations on the thermal decomposition of JP-10/iso-octane binary mixtures. *Fuel*, **2016**, 163, 148-156 12
- 50 The Interactions between Quaternary Ammonium Cationic Surfactants and Bovine Serum Albumin. *Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica*, **2016**, 32, 2951-2960 3.8 3
- 49 Enantioselective Total Synthesis of (+)-Steenkrotin A and Determination of Its Absolute Configuration. *Chemistry - A European Journal*, **2016**, 22, 959-70 4.8 9

48	Volumetric property of glycine, l-serine, l-alanine and l-proline in aqueous solutions of 1-phenylpiperazinium tetrafluoroborate. <i>Journal of Chemical Thermodynamics</i> , 2016 , 99, 75-81	2.9	23
47	Quantum interference effect of single-molecule conductance influenced by insertion of different alkyl length. <i>Electrochemistry Communications</i> , 2016 , 68, 86-89	5.1	11
46	Dehydrogenation of benzyl alcohol with NO as the hydrogen acceptor catalyzed by the rhodium(ii) carbene complex: insights from quantum chemistry calculations. <i>Dalton Transactions</i> , 2016 , 45, 16485-16491	4.3	9
45	Palladium(0)-Catalyzed Methylcyclopropanation of Norbornenes with Vinyl Bromides and Mechanism Study. <i>Organic Letters</i> , 2015 , 17, 3678-81	6.2	9
44	Explore the reaction mechanism of the Maillard reaction: a density functional theory study. <i>Journal of Molecular Modeling</i> , 2015 , 21, 132	2	5
43	Isolation, purification, and antioxidant activities of degraded polysaccharides from <i>Enteromorpha prolifera</i> . <i>International Journal of Biological Macromolecules</i> , 2015 , 81, 1026-30	7.9	53
42	Mechanistic insights into small molecule activation induced by ligand cooperativity in PCarbeneP nickel pincer complexes: a quantum chemistry study. <i>Journal of Molecular Modeling</i> , 2015 , 21, 242	2	10
41	Theoretically exploring the key role of the Lys412 residue in the conversion of N2O to N2 by nitrous oxide reductase from <i>Achromobacter cycloclastes</i> . <i>New Journal of Chemistry</i> , 2015 , 39, 8093-8099	2.6	3
40	[3+2] Redox-Neutral Cycloaddition of Nitrocyclopropanes with Styrenes by Visible-Light Photocatalysis. <i>Chemistry - A European Journal</i> , 2015 , 21, 9676-80	4.8	24
39	Novel Guanidinium-Based Ionic Liquids for Highly Efficient SO2 Capture. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 8054-62	3.4	30
38	Formation of Novel Aqueous Two-Phase Systems with Piperazinium-Based Ionic Liquids and Anionic Surfactants: Phase Behavior and Microstructure. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11798-806	3.4	7
37	Reaction Mechanisms of a TungstenTetramine Complex with One or Two Molecules of Alcohols and Arylaldehydes: A DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 1502-1511	2.3	6
36	Understanding the Reactivity Difference of Isocyanate and Isothiocyanate toward a Ruthenium Silylene Hydride Complex. <i>Organometallics</i> , 2014 , 33, 892-897	3.8	28
35	Pd-catalyzed bicyclization of 2-alkynylhalobenzenes and propargylic alcohols for the formation of indeno[1,2]furans: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2014 , 27, 237-244	2.1	3
34	Mechanism of Carbon Monoxide Induced N≡N Bond Cleavage of Nitrous Oxide Mediated by Molybdenum Complexes: A DFT Study. <i>Organometallics</i> , 2014 , 33, 1553-1562	3.8	7
33	Structure-function analysis of the conserved tyrosine and diverse π -stacking among class I histone deacetylases: a QM (DFT)/MM MD study. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3162-71	6.1	13
32	Mechanisms and reactivity differences for cycloaddition of anhydride to alkyne catalyzed by palladium and nickel catalysts: insight from density functional calculations. <i>Journal of Organic Chemistry</i> , 2014 , 79, 11911-21	4.2	28
31	Thermal Decomposition Kinetics and Mechanism of 1,1'-Bicyclohexyl. <i>Energy & Fuels</i> , 2014 , 28, 4523-4531	4.5	17

30	Conformational isomerism influence on the properties of piperazinium bis(trifluoromethylsulfonyl)imide. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 9085-95	3.4	9
29	An AIL/IL-based liquid/liquid extraction system for the purification of His-tagged proteins. <i>Applied Microbiology and Biotechnology</i> , 2014 , 98, 5665-75	5.7	10
28	A quantum chemistry study on thermochemical properties of high energy-density endothermic hydrocarbon fuel JP-10. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2183	2	9
27	Exploring the reaction mechanism of a cationic terminal iridium methylene complex with ethyl diazoacetate, a Lewis base and dihydrogen: a quantum chemistry study. <i>New Journal of Chemistry</i> , 2014 , 38, 4115	3.6	4
26	Mechanisms and origins of switchable regioselectivity of palladium- and nickel-catalyzed allene hydrosilylation with N-heterocyclic carbene ligands: a theoretical study. <i>Journal of Organic Chemistry</i> , 2014 , 79, 4517-27	4.2	47
25	DFT studies on the mechanisms of palladium-catalyzed intramolecular arylation of a silyl C(sp ³) π bond. <i>New Journal of Chemistry</i> , 2013 , 37, 2856	3.6	18
24	Theoretical studies on the reductive elimination reaction mechanism from neutral palladium(IV) sulfinate complexes. <i>Journal of Physical Organic Chemistry</i> , 2013 , 26, 933-938	2.1	8
23	A DFT study on the thermal cracking of JP-10. <i>Journal of Molecular Modeling</i> , 2013 , 19, 5355-65	2	8
22	Mechanism and Substrate-Dependent Rate-Determining Step in Palladium-Catalyzed Intramolecular Decarboxylative Coupling of Arenecarboxylic Acids with Aryl Bromides: A DFT Study. <i>Organometallics</i> , 2013 , 32, 6957-6968	3.8	18
21	A DFT study on palladium-catalyzed decarboxylative intramolecular aziridination reaction mechanism. <i>Journal of Organometallic Chemistry</i> , 2013 , 745-746, 417-422	2.3	10
20	DFT Studies on the Palladium-Catalyzed Dearomatization Reaction between Chloromethylnaphthalene and the Cyclic Amine Morpholine. <i>Organometallics</i> , 2013 , 32, 2336-2343	3.8	29
19	Radical Scavenging Activity of Myricetin. <i>Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica</i> , 2013 , 29, 1421-1432	3.8	9
18	Intermolecular interactions between gold clusters and selected amino acids cysteine and glycine: a DFT study. <i>Journal of Molecular Modeling</i> , 2012 , 18, 645-52	2	25
17	One-step cyclization: synthesis of N-heteroalkyl-N'-tosylpiperazines. <i>Journal of Organic Chemistry</i> , 2012 , 77, 7506-11	4.2	7
16	Explore the Catalytic Reaction Mechanism in the Reduction of NO by CO on the Rh ⁷⁺ Cluster: A Quantum Chemical Study. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 7776-7781	3.8	12
15	Oxygenolysis reaction mechanism of copper-dependent quercetin 2,3-dioxygenase: A density functional theory study. <i>Science China Chemistry</i> , 2012 , 55, 1832-1841	7.9	5
14	Understanding hydrogenation of the adenine-thymine base pairs and their anions: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 609-618	2.1	2
13	Nitric oxide adsorption and reduction reaction mechanism on the Rh ⁷⁽⁺⁾ cluster: a density functional theory study. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 14203-8	2.8	27

12	Enzymatic Reduction of Nitrate to Nitrite: Insight from Density Functional Calculations. <i>Organometallics</i> , 2010 , 29, 436-441	3.8	16
11	Osmapyridine and Osmapyridinium from a Formal [4+2] Cycloaddition Reaction. <i>Angewandte Chemie</i> , 2009 , 121, 5538-5542	3.6	26
10	Selective Synthesis of Osmanaphthalene and Osmanaphthalene by Intramolecular C-H Activation. <i>Angewandte Chemie</i> , 2009 , 121, 5569-5572	3.6	33
9	Osmapyridine and osmapyridinium from a formal [4+2] cycloaddition reaction. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5430-4	16.4	78
8	Selective synthesis of osmanaphthalene and osmanaphthalene by intramolecular C-H activation. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5461-4	16.4	93
7	Broad substrate specificity and catalytic mechanism of <i>Pseudomonas stutzeri</i> L-rhamnose isomerase: insights from QM/MM molecular dynamics simulations. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 11595-603	2.8	7
6	Combined quantum mechanics/molecular mechanics study on the reversible isomerization of glucose and fructose catalyzed by <i>Pyrococcus furiosus</i> phosphoglucose isomerase. <i>Journal of the American Chemical Society</i> , 2008 , 130, 7022-31	16.4	27
5	Exploring the interstitial atom in the FeMo cofactor of nitrogenase: insights from QM and QM/MM calculations. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 11435-9	3.4	25
4	Density functional study of protonation of deoxynucleosides: Electrophilic active sites and proton affinities. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 57-65	2.1	11
3	Effects of electron attachment on C5'-O5' and C1'-N1 bond cleavages of pyrimidine nucleotides: A theoretical study. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2025-32	3.5	10
2	Density functional study toward understanding dehydrogenation of the adenine-thymine base pair and its anion. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 4384-90	2.8	8
1	Electron attachment to the DNA bases adenine and guanine and dehydrogenation of their anionic derivatives: Density functional study. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 1261-1269	2.1	10