Ying Xue

List of Publications by Year
in descending order

192	4,145	134610	169272
papers	citations	34 h-index	56 g-index

196	196	196	5028
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Correction of gas adsorption capacity in quartz nanoslit and its application in recovering shale gas resources by CO2 injection: A molecular simulation. Energy, 2022, 240, 122789.	4.5	9
2	The dynamics of the fishing fleet in China Seas: A glimpse through AIS monitoring. Science of the Total Environment, 2022, 819, 153150.	3.9	17
3	A multispecies TAC approach to achieving long-term sustainability in multispecies mixed fisheries. ICES Journal of Marine Science, 2022, 79, 218-229.	1.2	5
4	Exploring the Effects of Water on the Mechanism of the Catalyst-Free Reaction between Isatin and 3-Methyl-2-pyrazolin-5-one from the Mixed Implicit/Explicit Multiple Types of Water Clusters. Journal of Physical Chemistry B, 2022, 126, 249-261.	1.2	1
5	Computational insight into the mechanism and stereoselectivity of cycloaddition between donorâ€“acceptor spirocyclopropane and aldehyde catalyzed by BrÃ¸nsted acid TsOH. Organic and Biomolecular Chemistry, 2022, 20, 4006-4015.	1.5	3
6	Theoretical Insights into Enantioselective [3 + 2] Cycloaddition between Cinnamaldehyde and Cyclic N-Sulfonyl Trifluoromethylated Ketimine Catalyzed by N-Heterocyclic Carbene. Journal of Physical Chemistry A, 2022, 126, 3124-3134.	1.1	1
7	Elucidating the mechanism and origins of selectivity on catalyst-dependent cyclization reactions to form polycyclic indolines from a theoretical study. RSC Advances, 2021, 11, 20622-20634.	1.7	1
8	Influence of water content on the [2Ïƒ+2Ïƒ+2Ï€] cycloaddition of dimethyl azodicarboxylate with quadricyclane in mixed methanolâ€“water solvents from QM/MM Monte Carlo simulations. Physical Chemistry Chemical Physics, 2021, 23, 20524-20532.	1.3	1
9	Evaluating the impacts of El NiÃ±o events on a marine bay ecosystem based on selected ecological network indicators. Science of the Total Environment, 2021, 763, 144205.	3.9	9
10	Application of TGFâ€Î²1, TIMPâ€‘1 and TIMPâ€‘2 small interfering RNAs can alleviate CCl4â€‘induced hepatic fibrosis in rats by rebalancing Th1/Th2 cytokines. Experimental and Therapeutic Medicine, 2021, 22, 963.	0.8	6
11	Mechanistic insight into B(C₆F₅)₃ catalyzed imine reduction with PhSiH₃ under stoichiometric water conditions. RSC Advances, 2021, 11, 20961-20969.	1.7	4
12	Insight into the Mechanism and Regioselectivity of Pd(OAc)2-Catalyzed Câ€“O Bond Activation via a Î²-O Elimination Approach: A Computational Study. Journal of Physical Chemistry A, 2021, 125, 9267-9278.	1.1	2
13	Mechanism and enantioselectivity of the asymmetric [3+2]-annulation between N-methylindole and enoldiazoacetamide catalyzed by prolinate-coordinated dirhodium: A theoretical study. Journal of Molecular Graphics and Modelling, 2020, 94, 107489.	1.3	2
14	The mechanism and diastereoselectivity in the formation of trifluoromethyl-containing spiro[pyrrolidin-3,2â€²-oxindole] by a catalyst-free and mutually activated [3+2]-cycloaddition reaction: a theoretical study. New Journal of Chemistry, 2020, 44, 17465-17476.	1.4	6
15	Insights into Câ€“O insertion in a carbene/alkyne metathesis cascade reaction catalyzed by Rh₂(OAc)₄: a DFT study. Catalysis Science and Technology, 2020, 10, 5513-5524.	2.1	2
16	Designing high-performance hypergolic propellants based on materials genome. Science Advances, 2020, 6, .	4.7	43
17	Computational insight into the mechanism and origin of high regioselectivity in the ring-opening cyclization of spirocyclopropanes with stabilized sulfonium ylides by the DFT. Journal of Molecular Modeling, 2020, 26, 255.	0.8	0
18	Computational Insight into the Mechanism of Mannich Reaction between Glycinate and Aryl Nâ€Diphenylphosphinyl Imine Catalyzed by Nâ€Quaternized Pyridoxal. ChemistrySelect, 2020, 5, 6504-6513.	0.7	3

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19	Super impact stable TATB explosives recrystallized by bicarbonate ionic liquids with a record solubility. Scientific Reports, 2020, 10, 4477.	1.6	23
20	Mechanistic insight into the optimal recovery efficiency of CBM in sub-bituminous coal through molecular simulation. Fuel, 2020, 266, 117137.	3.4	23
21	Insight into Adsorption of C₂H₂ and H₂ on Doped Graphene with Nonmetallic Atom (N, P, S): A Density Functional Theory Study. Journal of Nanoscience and Nanotechnology, 2020, 20, 1288-1295.	0.9	0
22	Prediction of matrix metal proteinases-12 inhibitors by machine learning approaches. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2627-2640.	2.0	9
23	Elucidating the origin of selectivity of [3â€‰+â€‰2]-cycloaddition reactions between thioketone and carbohydrate-derived nitrones by the DFT. Journal of Molecular Modeling, 2019, 25, 209.	0.8	8
24	A periodic density functional theory study of adsorption of CO₂ on anorthite (001) surface and effect of water. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950010.	1.8	5
25	Cataluminescence Coupled with Photoassisted Technology: A Highly Efficient Metal-Free Gas Sensor for Carbon Monoxide. Analytical Chemistry, 2019, 91, 13158-13164.	3.2	35
26	Computational insight into the mechanism and origins of high selectivities in the acylation of polyamines with 5-benzoyl-5-phenyl-1,5-dihydro-4H-pyrazol-4-one. Organic and Biomolecular Chemistry, 2019, 17, 140-150.	1.5	1
27	Role of Water in the Reaction Mechanism and endo / exo Selectivity of 1,3â€Dipolar Cycloadditions Elucidated by Quantum Chemistry and Machine Learning. Chemistry - A European Journal, 2019, 25, 8289-8303.	1.7	3
28	Effects of solvents on the DACBO-catalyzed vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole â€œon-waterâ€•and in solution from QM/MM MC simulations. RSC Advances, 2019, 9, 4932-4941.	1.7	5
29	Catalyst-Dependent Chemoselectivity in the Dirhodium-Catalyzed Cyclization Reactions Between Enodiazoacetamide and Nitrosoarene: A Theoretical Study. Frontiers in Chemistry, 2019, 7, 586.	1.8	6
30	Mechanism and Diastereoselectivity of [3+3] Cycloaddition between Enol Diazoacetate and Azomethine Imine Catalyzed by Dirhodium Tetracarboxylate: A Theoretical Study. European Journal of Organic Chemistry, 2018, 2018, 3086-3094.	1.2	14
31	DFT simulation on H2 adsorption over Ni-decorated defective h-BN nanosheets. Applied Surface Science, 2018, 439, 246-253.	3.1	67
32	Microsolvated Model for the Kinetics and Thermodynamics of Glycosidic Bond Dissociative Cleavage of Nucleoside D4G. Journal of Physical Chemistry B, 2018, 122, 1816-1825.	1.2	4
33	Theoretical Insights into Imidazolidine Oxidation of Imidacloprid by Cytochrome P450 3A4. Journal of Molecular Graphics and Modelling, 2018, 80, 173-181.	1.3	8
34	A theoretical study of UV-Vis spectrum and antioxidant activity of chryso-obtusin. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850015.	1.8	0
35	Mechanistic Insight into Hydrogen-Bond-Controlled Crystallinity and Adsorption Property of Covalent Organic Frameworks from Flexible Building Blocks. Chemistry of Materials, 2018, 30, 2299-2308.	3.2	208
36	Gas-phase alkyl and N-alkylamino cation affinities of anionic alpha-oxygen nucleophiles (H n XOâ˜; Xâ€‰=â€‰N,) Tj ETQq0 0 0 rgBT /O	0.8	1

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37	Adsorption of acetylene on ordered NixAg1-x/Ni (111) and effect of Ag-dopant: A DFT study. Applied Surface Science, 2018, 435, 521-528.	3.1	15
38	Computational Mechanism Study on Allylic Oxidation of cis-Internal Alkenes: Insight into the Lewis Acid-Assisted BrÃ¸nsted Acid (LBA) Catalysis in Heteroene Reactions. Journal of Organic Chemistry, 2018, 83, 13344-13355.	1.7	4
39	DFT investigation on the metabolic mechanisms of theophylline by cytochrome P450 monooxygenase. Journal of Molecular Graphics and Modelling, 2018, 84, 109-117.	1.3	8
40	Viscosity, Conductivity, and Electrochemical Property of Dicyanamide Ionic Liquids. Frontiers in Chemistry, 2018, 6, 59.	1.8	104
41	Enhancement of hydrogen sorption on metal(Ni, Rh, Pd) functionalized carbon nanotubes: a DFT study. Chemical Research in Chinese Universities, 2017, 33, 422-429.	1.3	7
42	The Role of Water in the Catalystâ€Free Aldol Reaction of Waterâ€Insoluble Nâ€Methylâ€2,4â€thiazolidinedione with Nâ€Methylisatin from QM/MM Monte Carlo Simulations. ChemPhysChem, 2017, 18, 2123-2131.	1.0	3
43	Comparison of DFT, MP2/CBS, and CCSD(T)/CBS methods for a dual-level QM/MM Monte Carlo simulation approach calculating the free energy of activation of reactions in solution and â€œon waterâ€: a case study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
44	Enhanced hydrogen storage on Li-doped defective graphene with B substitution: A DFT study. Applied Surface Science, 2017, 410, 166-176.	3.1	104
45	DFT study of the carbonation on mineral aerosol surface models of olivine: effect of water. Environmental Earth Sciences, 2017, 76, 1.	1.3	5
46	Enhanced interaction of nickel clusters with pyridinic-N (B) doped graphene using DFT simulation. Computational and Theoretical Chemistry, 2017, 1120, 8-16.	1.1	27
47	Toward Efficient CO₂ Capture Solvent Design by Analyzing the Effect of Chain Lengths and Amino Types to the Absorption Capacity, Bicarbonate/Carbamate, and Cyclic Capacity. Energy & Fuels, 2017, 31, 11099-11108.	2.5	38
48	Insight into substituent effects on the hydrolysis of amidines by a microhydration model. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	2
49	Influence Mechanisms of Rainfall and Terrain Characteristics on Total Nitrogen Losses from Regosol. Water (Switzerland), 2017, 9, 167.	1.2	9
50	Effects of Precipitation and Topography on Total Phosphorus Loss from Purple Soil. Water (Switzerland), 2017, 9, 315.	1.2	14
51	Fuzzy Comprehensive Assessment Method Based on the Entropy Weight Method and Its Application in the Water Environmental Safety Evaluation of the Heshangshan Drinking Water Source Area, Three Gorges Reservoir Area, China. Water (Switzerland), 2017, 9, 329.	1.2	61
52	Theoretical insight into the enhanced CH 4 desorption via H 2 O adsorption on different rank coal surfaces. Journal of Energy Chemistry, 2016, 25, 677-682.	7.1	30
53	Quantum chemical exploration on the metabolic mechanisms of caffeine by flavin-containing monooxygenase. Tetrahedron, 2016, 72, 2858-2867.	1.0	8
54	Theoretical elucidation of the metabolic mechanisms of phenothiazine neuroleptic chlorpromazine catalyzed by cytochrome P450 isoenzyme 1A2. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	6

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55	Molecular simulation of CH4, CO2, H2O and N2 molecules adsorption on heterogeneous surface models of coal. Applied Surface Science, 2016, 389, 894-905.	3.1	121
56	How Dirhodium Catalyst Controls the Enantioselectivity of [3 + 2]-Cycloaddition between Nitrone and Vinyldiazoacetate: A Density Functional Theory Study. Journal of Organic Chemistry, 2016, 81, 8082-8086.	1.7	12
57	Theoretical study on the metabolic mechanisms of levmepromazine by cytochrome P450. Journal of Molecular Modeling, 2016, 22, 237.	0.8	4
58	Insight Into the Influence of Ligand Conformation on Extraction Behaviour of Uranium: A Combined Theoretical and Experimental Study. Journal of Nanoscience and Nanotechnology, 2016, 16, 9603-9611.	0.9	0
59	Theoretical investigation on the structures and bonding properties of Pd(II), Pt(II) and Ni(II) complexes with tridentate CNC-pincer N-heterocyclic carbene ligands. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650037.	1.8	1
60	Theoretical study about effects of H2O and Na+ on adsorption of CO2 on kaolinite surfaces. Chemical Research in Chinese Universities, 2016, 32, 118-126.	1.3	6
61	Computational Mechanism Study of Catalyst-Dependent Competitive 1,2-Câ†'C, â^'Oâ†'C, and â^'Nâ†'C Migrations from Î²-Methylene-Î²-silyloxy-Î²-amido-Î±-diazoacetate: Insight into the Origins of Chemoselectivity. ACS Catalysis, 2016, 6, 162-175.	5.5	17
62	Effect of water on carbonation of mineral aerosol surface models of kaolinite: a density functional theory study. Environmental Earth Sciences, 2015, 73, 7053-7060.	1.3	12
63	Ligand-exchange mechanism: new insight into solid-phase extraction of uranium based on a combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 7214-7223.	1.3	34
64	Theoretical study on the N-demethylation mechanism of theobromine catalyzed by P450 isoenzyme 1A2. Journal of Molecular Graphics and Modelling, 2015, 61, 123-132.	1.3	13
65	Theoretical study on the mechanism of self-cleavage reaction of the glmS ribozyme. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	1
66	Cu-catalysed direct Câ€"H (hetero)arylation of [1,2,4]triazolo[4,3-a]pyridine to construct deep-blue-emitting luminophores. Organic and Biomolecular Chemistry, 2015, 13, 5372-5375.	1.5	24
67	Modeling, predicting and virtual screening of selective inhibitors of MMP-3 and MMP-9 over MMP-1 using random forest classification. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 30-40.	1.8	5
68	Metabolic mechanisms of caffeine catalyzed by cytochrome P450 isoenzyme 1A2: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	10
69	Predicting and Virtually Screening Breast Cancer Targeting Protein HEC1 Inhibitors by Molecular Descriptors and Machine Learning Methods. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 1795-1802.	2.2	3
70	CH₄, CO₂ and H₂OAdsorption on Nonmetallic Atom-Decorated Graphene Surfaces. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2014, 30, 251-256.	2.2	8
71	A theoretical exploration of the photoinduced reductive repair mechanisms of thymidine glycol. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 294, 88-95.	2.0	1
72	Effects of Edge Oxidation on the Stability and Halfâ€Metallicity of Graphene Quantum Dots. ChemPhysChem, 2014, 15, 157-164.	1.0	16

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73	Investigation of oxygen-containing group promotion effect on CO2â€“coal interaction by density functional theory. Applied Surface Science, 2014, 299, 162-169.	3.1	67
74	A Timeâ€Đependent DFT Study of the Absorption and Fluorescence Properties of Graphene Quantum Dots. ChemPhysChem, 2014, 15, 950-957.	1.0	92
75	A first-principle study of calcium-decorated BC2N sheet doped by boron or carbon for high hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 9307-9320.	3.8	36
76	Medium Effects on the 1,3-Dipolar Cycloaddition of Pyridazinium Dicyanomethanide with Ethyl Vinyl Ketone in Pure and Mixed Solvents from QM/MM Simulations. Journal of Organic Chemistry, 2014, 79, 4863-4870.	1.7	7
77	Tuning Hydrogen Storage in Lithiumâ€Functionalized BC₂N Sheets by Doping with Boron and Carbon. ChemPhysChem, 2014, 15, 3015-3025.	1.0	11
78	Cooperation between the surface hydroxyl groups of Ruâ€“SiO₂@mSiO₂and water for good catalytic performance for hydrogenation of quinoline. Catalysis Science and Technology, 2014, 4, 1939-1948.	2.1	57
79	Mechanistic insights into <scp>l</scp>-proline-catalyzed transamidation of carboxamide with benzylamine from density functional theory calculations. RSC Advances, 2014, 4, 30108-30117.	1.7	13
80	Mechanism and regioselectivity of the cycloaddition between nitrone and dirhodium vinylcarbene catalyzed by Rh2(O2CH)4: a computational study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	7
81	Mechanism for the decomposition of 5-aza-2â€²-deoxycytidine: a theoretical study using Monte Carlo simulation plus local microhydration model. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	1
82	Stimulation of Nâ^'glycoside transfer in deoxythymidine glycol: mechanism of the initial step in base excision repair. Journal of Molecular Modeling, 2014, 20, 2168.	0.8	1
83	Adsorption of HCN on reduced graphene oxides: a firstâ€“principles study. Journal of Molecular Modeling, 2014, 20, 2214.	0.8	25
84	Theoretical calculations of the pK a values of 1-aryl-4-propylpiperazine drugs in aqueous solution. Chemical Research in Chinese Universities, 2014, 30, 455-460.	1.3	2
85	Predicting and Virtually Screening the Selective Inhibitors of MMP-13 over MMP-1 by Molecular Descriptors and Machine Learning Methods. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2014, 30, 171-182.	2.2	1
86	QM/MM investigation on 1,3-dipolar cycloadditions of the phthalazinium dicyanomethanide with three different dipolarophiles on water and in solution. Physical Chemistry Chemical Physics, 2013, 15, 11846.	1.3	8
87	Quantitative structureâ€“activity relationship study of influenza virus neuraminidase A/PR/8/34 (H1N1) inhibitors by genetic algorithm feature selection and support vector regression. Chemometrics and Intelligent Laboratory Systems, 2013, 127, 35-42.	1.8	23
88	Quantum chemical studies on adsorption of CO2 on nitrogen-containing molecular segment models of coal. Surface Science, 2013, 616, 85-92.	0.8	34
89	Adsorption of CH4 on nitrogen- and boron-containing carbon models of coal predicted by density-functional theory. Applied Surface Science, 2013, 285, 190-197.	3.1	62
90	Experimental and theoretical investigation on the interaction between palladium nanoparticles and functionalized carbon nanotubes for Heck synthesis. Catalysis Today, 2013, 212, 206-214.	2.2	42

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91	Theoretical study on the aminolysis of p-substituted phenyl acetates with dimeric ammonia in vacuo and acetonitrile. Computational and Theoretical Chemistry, 2013, 1008, 8-14.	1.1	11
92	In silico prediction of spleen tyrosine kinase inhibitors using machine learning approaches and an optimized molecular descriptor subset generated by recursive feature elimination method. Computers in Biology and Medicine, 2013, 43, 395-404.	3.9	17
93	MECHANISMS FOR THE DECOMPOSITION OF HYDROXYL-RADICAL-INDUCED CYTOSINE HYDROPEROXIDES: A COMPUTATIONAL STUDY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350027.	1.8	2
94	Quantitative Structure-Activity Relationship Study of the Non-Nucleoside Inhibitors of HCV NS5B Polymerase by Machine Learning Methods. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 1639-1647.	2.2	1
95	Classification Prediction of Inhibitors of H1N1 Neuraminidase by Machine Learning Methods. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 217-223.	2.2	2
96	In Silico Prediction of Adverse Drug Reactions and Toxicities Based on Structural, Biological and Clinical Data. Current Drug Safety, 2012, 7, 225-237.	0.3	1
97	THEORETICAL STUDY ON CUI-CATALYZED LIGAND-FREE N-ARYLATION OF IMIDAZOLE WITH BROMOBENZENE. Journal of Theoretical and Computational Chemistry, 2012, 11, 1135-1147.	1.8	9
98	THEORETICAL INVESTIGATIONS ON THE MECHANISM OF ACTIVATION OF AMMONIA BY A p-DIMETHYLAMINOPYRIDINE COORDINATED SI=O DOUBLE BOND. Journal of Theoretical and Computational Chemistry, 2012, 11, 437-481.	1.8	1
99	Copper(II)-Catalyzed Dehydrogenative Cross-Coupling between Two Azoles. Journal of Organic Chemistry, 2012, 77, 7677-7683.	1.7	88
100	Investigation of the doped transition metal promotion effect on CO2 chemisorption on Ni (111). Applied Surface Science, 2012, 258, 6239-6245.	3.1	17
101	A general acidâ€“general base reaction mechanism for human brain aspartoacylase: A QM/MM study. Computational and Theoretical Chemistry, 2012, 980, 85-91.	1.1	8
102	Adsorption of methane on carbon models of coal surface studied by the density functional theory including dispersion correction (DFT-D3). Computational and Theoretical Chemistry, 2012, 992, 37-47.	1.1	55
103	A DFT study of methane activation on graphite surfaces with vacancy defects. Journal of Natural Gas Chemistry, 2012, 21, 708-712.	1.8	26
104	Ligand-switching and counteranion-induced hierarchical self-assembly of silver-NHC complexes. Chemical Science, 2012, 3, 359-363.	3.7	36
105	Theoretical study of static (Hyper)polarizabilities of twisted intramolecular charge transfer chromophores. International Journal of Quantum Chemistry, 2012, 112, 1086-1096.	1.0	6
106	Role of bifunctional catalyst 2-pyridone in the aminolysis of p-nitrophenyl acetate with n-butylamine: A computational study. Journal of Molecular Catalysis A, 2012, 355, 102-112.	4.8	12
107	Mechanism for the reaction of 2â€naphthol with Nâ€methylâ€Nâ€phenylâ€hydrazine suggested by the density functional theory investigations. Journal of Computational Chemistry, 2012, 33, 220-230.	1.5	6
108	Sulfurâ€“Nitrogen and Carbonâ€“Nitrogen Bond Formation by Intermolecular Imination and Amidation without Catalyst. European Journal of Organic Chemistry, 2012, 2012, 1554-1562.	1.2	17

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109	Theoretical studies on the chemical decomposition of 5-aza-2â€²-deoxycytidine: DFT study and Monte Carlo simulation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	3
110	A DFT Study of Methane Adsorption on Nitrogen-Containing Organic Heterocycles. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2012, 28, 1101-1106.	2.2	11
111	Integration of Ligand-Based and Structure-Based Approaches for Virtual Screening of Factor Xa Inhibitors. , 2012, , 141-154.		0
112	Quantum mechanics study and Monte Carlo simulation on the hydrolytic deamination of 5-methylcytosine glycol. Physical Chemistry Chemical Physics, 2011, 13, 6471.	1.3	9
113	Substituent Effect on the Acid-Promoted Hydrolysis of 2-Aryloxazolin-5-one: Normal vs Reverse. Journal of Physical Chemistry A, 2011, 115, 4995-5004.	1.1	6
114	Theoretical Investigations on the Mechanism of Benzoin Condensation Catalyzed by Pyrido[1,2-a]-2-ethyl[1,2,4]triazol-3-ylidene. Journal of Physical Chemistry A, 2011, 115, 1408-1417.	1.1	36
115	Effect of training data size and noise level on support vector machines virtual screening of genotoxic compounds from large compound libraries. Journal of Computer-Aided Molecular Design, 2011, 25, 455-467.	1.3	3
116	QM/MM study on catalytic mechanism of aspartate racemase from Pyrococcus horikoshii OT3. Theoretical Chemistry Accounts, 2011, 129, 781-791.	0.5	4
117	A quantitative analysis of intramolecular charge transfer contribution to polarizability responses in donor-Ï€-acceptor molecules. Chemical Physics Letters, 2011, 511, 12-15.	1.2	4
118	QSAR study for cytotoxicity of diterpenoid tanshinones. Interdisciplinary Sciences, Computational Life Sciences, 2011, 3, 121-127.	2.2	5
119	Reexamination of the Ï€â€bond strengths within H₂C=XH_n systems: A theoretical study. Journal of Computational Chemistry, 2011, 32, 1361-1367.	1.5	5
120	AB INITIO COMPUTATIONAL INVESTIGATIONS ON THE GAS-PHASE HOMODIMERIZATION AND KETO-ENOL TAUTOMERISM OF THE MONOCHALCOGENOCARBOXYLIC ACIDS CH3C(=O)XH (X = S, Se, Te). Journal of Theoretical and Computational Chemistry, 2011, 10, 41-51.	1.8	4
121	In silico prediction and screening of Î³â€secretase inhibitors by molecular descriptors and machine learning methods. Journal of Computational Chemistry, 2010, 31, 1249-1258.	1.5	22
122	Theoretical studies on the gas-phase pyrolysis of 2-trimethylsilylethanol. Computational and Theoretical Chemistry, 2010, 941, 127-132.	1.5	1
123	Molecular dynamics and density functional theory studies of substrate binding and catalysis of human brain aspartoacylase. Journal of Molecular Graphics and Modelling, 2010, 28, 799-806.	1.3	10
124	Mechanisms of norbornadiene dimerization to Binorâ€<scp>S</scp> using cationic Co^I, Rh^I, and Ir^I catalysts. Journal of Computational Chemistry, 2010, 31, 2248-2257.	1.5	5
125	Selfâ€Assembly of Discrete Homochiral, Helical, Hydrogenâ€Bonded Nanocages: From Vesicles to Microspheres and Tubules Capable of Gelating Solvents. Chemistry - A European Journal, 2010, 16, 2250-2257.	1.7	16
126	Theoretical study on the aminolysis of ester catalyzed by TBD: Hydrogen bonding or covalent bonding of the catalyst?. Computational and Theoretical Chemistry, 2010, 942, 137-144.	1.5	12

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127	Identification of vasodilators from molecular descriptors by machine learning methods. Chemometrics and Intelligent Laboratory Systems, 2010, 101, 95-101.	1.8	2
128	Prediction of acetylcholinesterase inhibitors and characterization of correlative molecular descriptors by machine learning methods. European Journal of Medicinal Chemistry, 2010, 45, 1167-1172.	2.6	32
129	Theoretical Investigations on the Thermal Decomposition Mechanism of 5-Hydroxy-6-hydroperoxy-5,6-dihydrothymidine in Water. Journal of Physical Chemistry B, 2010, 114, 12641-12654.	1.2	18
130	Mechanism Insight into the Cyanide-Catalyzed Benzoin Condensation: A Density Functional Theory Study. Journal of Physical Chemistry A, 2010, 114, 9222-9230.	1.1	24
131	Copper-catalyzed decarboxylative cross-coupling of alkynyl carboxylic acids with aryl halides. Chemical Communications, 2010, 46, 9049.	2.2	119
132	THE INFLUENCES OF OXIDATION AND CATIONIZATION ON THE N-GLYCOSIDIC BOND STABILITY OF 8-OXO-2â€²-DEOXYADENOSINE â€" A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2009, 08, 1253-1264.	1.8	6
133	Comparative Analysis of Machine Learning Methods in Ligand-Based Virtual Screening of Large Compound Libraries. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 344-357.	0.6	62
134	THEORETICAL STUDY ON THE STRUCTURE TRANSFORMATIONS OF CRYPTOTANSHINONE AND TANSHINONE I WITH HYDRION OR HYDROXIDE ION. Journal of Theoretical and Computational Chemistry, 2009, 08, 203-213.	1.8	1
135	Prediction of antibacterial compounds by machine learning approaches. Journal of Computational Chemistry, 2009, 30, 1202-1211.	1.5	49
136	Prediction of novel and selective TNF-alpha converting enzyme (TACE) inhibitors and characterization of correlative molecular descriptors by machine learning approaches. Journal of Molecular Graphics and Modelling, 2009, 28, 236-244.	1.3	19
137	Theoretical Studies on the Water-Assisted Hydrolysis of N,N-Dimethyl-Nâ€²-(2â€²,3â€²-dideoxy-3â€²-thiacytidine) Formamidine with Three Water Molecules. Journal of Physical Chemistry A, 2009, 113, 325-331.	1.1	12
138	Effects of Substituent and Leaving Group on the Gas-Phase SN2 Reactions of Phenoxides with Halomethanes: A DFT Investigation. Journal of Physical Chemistry A, 2009, 113, 10359-10366.	1.1	12
139	Ultrasound-Induced Switching of Sheetlike Coordination Polymer Microparticles to Nanofibers Capable of Gelating Solvents. Journal of the American Chemical Society, 2009, 131, 1689-1691.	6.6	113
140	Theoretical Studies on the Thermodynamics and Kinetics of the N-Glycosidic Bond Cleavage in Deoxythymidine Glycol. Journal of Physical Chemistry B, 2009, 113, 10409-10420.	1.2	26
141	A support vector machines approach for virtual screening of active compounds of single and multiple mechanisms from large libraries at an improved hit-rate and enrichment factor. Journal of Molecular Graphics and Modelling, 2008, 26, 1276-1286.	1.3	76
142	The substituent effects of the leaving groups on the aminolysis of phenyl acetates: DFT studies. Chemical Physics, 2008, 345, 73-81.	0.9	17
143	Theoretical study on the hydrolysis mechanism of N,N-dimethyl-Nâ€²-(2â€²,3â€²-dideoxy-3â€²-thiacytidine)formamidine. Science in China Series B: Chemistry, 2008, 51, 911-917.	0.8	3
144	Identifying hERG Potassium Channel Inhibitors by Machine Learning Methods. QSAR and Combinatorial Science, 2008, 27, 1028-1035.	1.5	16

#	Article	IF	Citations
145	Theoretical study on the hydrolysis mechanism of N,Nâ€dimethylâ€Nâ€²â€(2â€oxoâ€1,) Tj ETQq1 1 0.784314 rgBT /Over Computational Chemistry, 2008, 29, 1222-1232.	1.5	21
146	Computational studies on the dimers and the thermal dimerization of norbornadiene. Journal of Computational Chemistry, 2008, 29, 1250-1258.	1.5	6
147	The effects of oxidation and protonation on the N-glycosidic bond stability of 8-oxo-2â€²-deoxyguanosine: DFT study. Computational and Theoretical Chemistry, 2008, 860, 52-57.	1.5	13
148	Computational study on 1,1,3,3-tetramethylguanidine-catalyzed cyanosilylation mechanism of hypnone. Computational and Theoretical Chemistry, 2008, 863, 60-65.	1.5	0
149	Water-assisted enol-to-keto tautomerism of a simple peptide model: A computational investigation. Computational and Theoretical Chemistry, 2008, 868, 55-64.	1.5	16
150	Computational Study on the Aminolysis of Î²-Hydroxy-Î±,Î²-Unsaturated Ester via the Favorable Path Including the Formation of Î±-Oxo Ketene Intermediate. Journal of Physical Chemistry A, 2008, 112, 4501-4510.	1.1	14
151	Evaluation of Virtual Screening Performance of Support Vector Machines Trained by Sparsely Distributed Active Compounds. Journal of Chemical Information and Modeling, 2008, 48, 1227-1237.	2.5	41
152	DFT Study and Monte Carlo Simulation on the Aminolysis of XC(O)OCH₃ (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 T Theory and Computation, 2008, 4, 1643-1653.	2.3	18
153	Theoretical Study of the Acid-Promoted Hydrolysis of Oxazolin-5-one: A Microhydration Model. Journal of Physical Chemistry B, 2008, 112, 10659-10667.	1.2	16
154	Theoretical Studies on the Hydrolysis Mechanism of N-(2-oxo-1,2-dihydro-pyrimidinyl) Formamide. Journal of Physical Chemistry B, 2007, 111, 2357-2364.	1.2	25
155	MODELâ€"molecular descriptor lab: A web-based server for computing structural and physicochemical features of compounds. Biotechnology and Bioengineering, 2007, 97, 389-396.	1.7	50
156	Machine learning approaches for predicting compounds that interact with therapeutic and ADMET related proteins. Journal of Pharmaceutical Sciences, 2007, 96, 2838-2860.	1.6	54
157	Density functional theory studies on conformational stability and vibrational spectra of 2â€²-deoxyinosine. Computational and Theoretical Chemistry, 2007, 802, 35-44.	1.5	11
158	Density functional theory investigations on the conformational stability and vibrational spectra of the model compound of vitamin K. Computational and Theoretical Chemistry, 2007, 820, 40-47.	1.5	10
159	Prediction of factor Xa inhibitors by machine learning methods. Journal of Molecular Graphics and Modelling, 2007, 26, 505-518.	1.3	28
160	A theoretical investigation on the geometry and vibrational spectra of 10,10,2,6,5-pentamethyl-1-hydroxychroman: A model of Î±-tocopherol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 1287-1295.	2.0	6
161	Modeling of Hydrogen Bonds in Monohydrated 2,4-Dithiothymine:â€‰ An Ab Initio and AIM Study. Journal of Physical Chemistry B, 2006, 110, 1416-1422.	1.2	3
162	Classification of a Diverse Set of Tetrahymena pyriformis Toxicity Chemical Compounds from Molecular Descriptors by Statistical Learning Methods. Chemical Research in Toxicology, 2006, 19, 1030-1039.	1.7	75

#	Article	IF	Citations
163	Comprehensive mechanistic study of ion pair SN2 reactions of lithium isocyanate and methyl halides. International Journal of Quantum Chemistry, 2006, 106, 1653-1663.	1.0	2
164	Ab initio potential energy surface and predicted microwave spectra for Arï£¿OCS dimer and structures of Arnï£¿OCS (n = 2â€“14) clusters. Journal of Computational Chemistry, 2006, 27, 1045-1053.	1.5	17
165	Application of Support Vector Machines to In Silico Prediction of Cytochrome P450 Enzyme Substrates and Inhibitors. Current Topics in Medicinal Chemistry, 2006, 6, 1593-1607.	1.0	28
166	Prediction of Compounds with Specific Pharmacodynamic, Pharmacokinetic or Toxicological Property by Statistical Learning Methods. Mini-Reviews in Medicinal Chemistry, 2006, 6, 449-459.	1.1	23
167	DFT study and Monte Carlo simulation on proton transfers of 2-amino-2-oxazoline, 2-amino-2-thiazoline, and 2-amino-2-imidazoline in the gas phase and in water. Journal of Computational Chemistry, 2005, 26, 994-1005.	1.5	17
168	Statistical learning approach for predicting specific pharmacodynamic, pharmacokinetic, or toxicological properties of pharmaceutical agents. Drug Development Research, 2005, 66, 245-259.	1.4	25
169	Prediction of Genotoxicity of Chemical Compounds by Statistical Learning Methods. Chemical Research in Toxicology, 2005, 18, 1071-1080.	1.7	77
170	A Computational Study on the Mechanism for the Chemical Fixation of Nitric Oxide Leading to 1,2,3-Oxadiazole 3-oxide. Journal of Organic Chemistry, 2005, 70, 5045-5054.	1.7	3
171	Effect of Selection of Molecular Descriptors on the Prediction of Bloodâ^'Brain Barrier Penetrating and Nonpenetrating Agents by Statistical Learning Methods. Journal of Chemical Information and Modeling, 2005, 45, 1376-1384.	2.5	145
172	Prediction of Torsade-Causing Potential of Drugs by Support Vector Machine Approach No funding was used to assist in conducting the study and the authors do not have any conflicts of interest directly relevant to the contents of the manuscript.. Toxicological Sciences, 2004, 79, 170-177.	1.4	71
173	MoViES: molecular vibrations evaluation server for analysis of fluctuational dynamics of proteins and nucleic acids. Nucleic Acids Research, 2004, 32, W679-W685.	6.5	14
174	A theoretical study of solvent effects on tautomerism and electronic absorption spectra of 3-hydroxy-2-mercaptopyridine and 2,3-dihydroxypyridine. Journal of Computational Chemistry, 2004, 25, 1833-1839.	1.5	27
175	Ab initio investigation on the structure and vibrational frequencies of Ne2â€“OCS trimer. Computational and Theoretical Chemistry, 2004, 684, 61-65.	1.5	1
176	Effect of Molecular Descriptor Feature Selection in Support Vector Machine Classification of Pharmacokinetic and Toxicological Properties of Chemical Agents. Journal of Chemical Information and Computer Sciences, 2004, 44, 1630-1638.	2.8	149
177	Prediction of P-Glycoprotein Substrates by a Support Vector Machine Approach. Journal of Chemical Information and Computer Sciences, 2004, 44, 1497-1505.	2.8	158
178	Effects of Substituents and Solvents on the Reactions of Iminophosphorane with Formaldehyde:Ab InitioMO Calculation and Monte Carlo Simulation. Journal of Physical Chemistry A, 2003, 107, 7945-7951.	1.1	17
179	Ab initio studies for the photodissociation mechanism of hydroxyacetone. Journal of Computational Chemistry, 2003, 24, 931-938.	1.5	10
180	Theoretical studies on the gas-phase pyrolysis of 2-phenoxycarboxylic acids: An ONIOM approach. Journal of Computational Chemistry, 2003, 24, 963-972.	1.5	8

#	Article	IF	Citations
181	Theoretical Study of the aza-Wittig Reactions of X3PNH (X=H and Cl) with Formaldehyde in Gas Phase and in Solution. Journal of Physical Chemistry A, 2002, 106, 9053-9058.	1.1	16
182	Density functional theory studies on the structures and vibrational spectra of 3,6-dichlorocarbazole and 3,6-dibromocarbazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 2227-2235.	2.0	6
183	Density functional theory studies on molecular structure and IR spectra of 9-methyladenine: A scaled quantum mechanical force field approach. International Journal of Quantum Chemistry, 2000, 76, 686-699.	1.0	42
184	Density functional theory studies on tautomeric stability and infrared spectra of 2-chloroadenine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2000, 56, 1929-1938.	2.0	16
185	Density functional theory study on fundamental vibrational spectra of disilyl iodide and its isotopomer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2000, 56, 567-574.	2.0	1
186	Computational studies of the structure and vibrational spectra of hexafluorodisilane. Computational and Theoretical Chemistry, 1999, 469, 151-156.	1.5	1
187	Theoretical studies of force fields and IR spectra of isocytosine. International Journal of Quantum Chemistry, 1999, 72, 53-60.	1.0	14
188	Density Functional Theory Studies on Vibrational Spectra of Si2H5X (X = F, Cl, Br) and Their Isotopomers. Journal of Physical Chemistry A, 1999, 103, 7437-7444.	1.1	1
189	Ab Initio Study on the Vibrational Spectrum of Fluorine Fluorosulfate. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 1999, 15, 138-142.	2.2	0
190	Ab initio studies on vibrational spectra of XSO2NCO (X = F,Cl): harmonic force fields and frequency assignments. Science in China Series B: Chemistry, 1998, 41, 91-96.	0.8	6
191	THE METHOD OF KINEMATICALLY DEFINED FORCE CONSTANTS IN MOLECULAR VIBRATION. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 1986, 2, 505-511.	2.2	0
192	Elucidating the mechanism and reactivity of the reaction between the donorâ€“acceptorâ€“acceptor 1,3-bisdiazo compound and cinnamyl alcohol catalyzed by Rh2(OAc)4: a DFT study. New Journal of Chemistry, 0, , .	1.4	0