Shu-Hua Li

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/840262/publications.pdf

Version: 2024-02-01

232 papers	8,916 citations	41344 49 h-index	56724 83 g-index
248 all docs	248 docs citations	248 times ranked	7655 citing authors

#	Article	IF	Citations
1	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. Physical Chemistry Chemical Physics, 2022, 24, 1326-1337.	2.8	18
2	Mechanistic Insight into Hydroboration of Imines from Combined Computational and Experimental Studies. Chemistry - A European Journal, 2022, 28, .	3.3	8
3	Iodoperfluoroalkylation of unactivated alkenes via pyridine-boryl radical initiated atom-transfer radical addition. Organic and Biomolecular Chemistry, 2022, 20, 2857-2862.	2.8	8
4	Structures and properties of ionic crystals and condensed phase ionic liquids predicted with the generalized energyâ€based fragmentation method. Journal of Computational Chemistry, 2022, 43, 704-716.	3.3	6
5	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. Chinese Journal of Chemical Physics, 2022, 35, 167-176.	1.3	3
6	Transition orbital projection approach for excited state tracking. Journal of Chemical Physics, 2022, 156, .	3.0	2
7	Electroâ€Descriptors for the Performance Prediction of Electroâ€Organic Synthesis. Angewandte Chemie, 2021, 133, 4245-4253.	2.0	13
8	Electroâ€Descriptors for the Performance Prediction of Electroâ€Organic Synthesis. Angewandte Chemie - International Edition, 2021, 60, 4199-4207.	13.8	35
9	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. Accounts of Chemical Research, 2021, 54, 169-181.	15.6	36
10	Borane-catalyzed selective dihydrosilylation of terminal alkynes: reaction development and mechanistic insight. Chemical Science, 2021, 12, 10883-10892.	7.4	13
11	Rational design of the nickelâ€borane complex for efficient hydrogenation of styrene. Journal of Computational Chemistry, 2021, 42, 545-551.	3.3	1
12	From helices to superhelices: hierarchical assembly of homochiral van der Waals 1D coordination polymers. Chemical Science, 2021, 12, 12619-12630.	7.4	9
13	Controlled Fluorescence Enhancement of DNA-Binding Dye Through Chain Length Match between Oligoguanine and TOTO. Journal of Physical Chemistry B, 2021, 125, 518-527.	2.6	4
14	B(C₆F₅)₃-Catalyzed Sequential Additions of Terminal Alkynes to para-Substituted Phenols: Selective Construction of Congested Phenol-Substituted Quaternary Carbons. Organic Letters, 2021, 23, 5533-5538.	4.6	10
15	B(C₆F₅)₃â€Catalyzed Hydroarylation of Aryl Alkynes for the Synthesis of 1,1â€Diaryl and Triaryl Substituted Alkenes. European Journal of Organic Chemistry, 2021, 2021, 5238-5242.	2.4	4
16	Mechanistic insights into the dearomative diborylation of pyrazines: a radical or non-radical process?. Dalton Transactions, 2021, 50, 6982-6990.	3.3	8
17	Generalized energy-based fragmentation approach for calculations of solvation energies of large systems. Physical Chemistry Chemical Physics, 2021, 23, 19394-19401.	2.8	8
18	Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. Journal of Chemical Theory and Computation, 2021, 17, 756-766.	5.3	32

#	Article	IF	Citations
19	An Efficient Approach for 3,3-Disubstituted Oxindoles Synthesis: Aryl Iodine Catalyzed Intramolecular Câ€“N Bond Oxidative Cross-Coupling. Organic Letters, 2021, 23, 8750-8754.	4.6	12
20	Computational and data driven molecular material design assisted by low scaling quantum mechanics calculations and machine learning. Chemical Science, 2021, 12, 14987-15006.	7.4	16
21	Catalytic Dehydrogenation of Ammonia Borane Mediated by a Pt(0)/Borane Frustrated Lewis Pair: Theoretical Design. ChemPhysChem, 2020, 21, 2573-2578.	2.1	7
22	B(C₆F₅)₃â€Catalyzed Tandem Friedelâ€Crafts and Cå^'H/Cå^'O Coupling Reactions of Dialkylanilines. Chemistry - an Asian Journal, 2020, 15, 3082-3086.	3.3	6
23	Enantioselective copper-catalysed defluorosilylation of trifluoro-methylated alkenes with silylboronates. Organic Chemistry Frontiers, 2020, 7, 2618-2627.	4.5	34
24	Describing Strong Correlation with Block-Correlated Coupled Cluster Theory. Journal of Physical Chemistry Letters, 2020, 11, 7536-7543.	4.6	12
25	Automatic Selection of Active Orbitals from Generalized Valence Bond Orbitals. Journal of Physical Chemistry A, 2020, 124, 8321-8329.	2.5	14
26	Metal-free reductive coupling of aliphatic aldehydes/ketones with 4-cyanopyridines: expanded scope and mechanistic studies. Organic Chemistry Frontiers, 2020, 7, 2744-2751.	4.5	24
27	Preface: Celebrating the 100th anniversary of chemical sciences in Nanjing University. Science China Chemistry, 2020, 63, 561-563.	8.2	0
28	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. Journal of Physical Chemistry A, 2020, 124, 5007-5014.	2.5	23
29	Selective Quadruple C(sp3)-F Functionalization of Polyfluoroalkyl Ketones. IScience, 2020, 23, 101259.	4.1	27
30	Targeted tumour theranostics in mice via carbon quantum dots structurally mimicking large amino acids. Nature Biomedical Engineering, 2020, 4, 704-716.	22.5	243
31	H₂ Activation by Heterobimetallic Gold(I)/Platinum(0) Complex: Theoretical Understanding of Electronic Processes and Prediction on More Active Species. Journal of Physical Chemistry C, 2020, 124, 4525-4533.	3.1	5
32	Photoredoxâ€Controlled Î²â€Regioselective Radical Hydroboration of Activated Alkenes with NHCâ€Boranes. Angewandte Chemie - International Edition, 2020, 59, 12817-12821.	13.8	46
33	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2020, 16, 2995-3005.	5.3	19
34	Focus on electronic structure theory in China. Electronic Structure, 2020, 2, 020201.	2.8	0
35	Transitionâ€Metalâ€Free Defluorosilylation of Fluoroalkenes with Silylboronates. Chinese Journal of Chemistry, 2019, 37, 1009-1014.	4.9	49
36	Dextran as an elicitor of phenylpropanoid and flavonoid biosynthesis in tomato fruit against gray mold infection. Carbohydrate Polymers, 2019, 225, 115236.	10.2	12

#	Article	IF	Citations
37	The antibiotic activity and mechanisms of active metabolites (Streptomyces alboflavus TD-1) against Ralstonia solanacearum. Biotechnology Letters, 2019, 41, 1213-1222.	2.2	4
38	Mechanistic Insight Into the AuCN Catalyzed Annulation Reaction of Salicylaldehyde and Aryl Acetylene: Cyanide Ion Promoted Umpolung Hydroacylation/Intramolecular Oxa-Michael Addition Mechanism. Frontiers in Chemistry, 2019, 7, 557.	3.6	3
39	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of N-Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. ACS Catalysis, 2019, 9, 10142-10151.	11.2	42
40	Cooperative Au/Ag Dual-Catalyzed Cross-Dehydrogenative Biaryl Coupling: Reaction Development and Mechanistic Insight. Journal of the American Chemical Society, 2019, 141, 3187-3197.	13.7	101
41	Perfluoroalkylative pyridylation of alkenesvia4-cyanopyridine-boryl radicals. Chemical Science, 2019, 10, 2767-2772.	7.4	81
42	N-Centered Chiral Self-Sorting and Supramolecular Helix of TrÃ¶ger's Base-Based Dimeric Macrocycles in Crystalline State. Frontiers in Chemistry, 2019, 7, 383.	3.6	10
43	Analytical Energy Gradients for the Cluster-in-Molecule MP2 Method and Its Application to Geometry Optimizations of Large Systems. Journal of Chemical Theory and Computation, 2019, 15, 3623-3634.	5.3	11
44	Chemoselective Boraneâ€Catalyzed Hydroarylation of 1,3â€Dienes with Phenols. Angewandte Chemie, 2019, 131, 1708-1713.	2.0	7
45	Cluster-in-Molecule Local Correlation Approach for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 2933-2943.	5.3	14
46	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. Physical Chemistry Chemical Physics, 2019, 21, 4072-4081.	2.8	19
47	Transcriptomic Insights into Benzenamine Effects on the Development, Aflatoxin Biosynthesis, and Virulence of Aspergillus flavus. Toxins, 2019, 11, 70.	3.4	12
48	Depression of Fungal Polygalacturonase Activity in Solanum lycopersicum Contributes to Antagonistic Yeast-Mediated Fruit Immunity to Botrytis. Journal of Agricultural and Food Chemistry, 2019, 67, 3293-3304.	5.2	11
49	Improved generalized energy-based fragmentation approach and its applications to the binding energies of supramolecular complexes. Electronic Structure, 2019, 1, 044003.	2.8	8
50	Fully optimized implementation of the clusterâ€inâ€molecule local correlation approach for electron correlation calculations of large systems. Journal of Computational Chemistry, 2019, 40, 1130-1140.	3.3	24
51	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems. Journal of Chemical Theory and Computation, 2019, 15, 141-153.	5.3	19
52	Chemoselective Boraneâ€Catalyzed Hydroarylation of 1,3â€Dienes with Phenols. Angewandte Chemie - International Edition, 2019, 58, 1694-1699.	13.8	54
53	Organocatalytic reductive coupling of aldehydes with 1,1-diarylethylenes using an in situ generated pyridine-boryl radical. Chemical Science, 2018, 9, 3664-3671.	7.4	56
54	Accurate prediction of the structure and vibrational spectra of ionic liquid clusters with the generalized energy-based fragmentation approach: critical role of ion-pair-based fragmentation. Physical Chemistry Chemical Physics, 2018, 20, 13547-13557.	2.8	18

#	Article	IF	Citations
55	THz spectra and corresponding vibrational modes of DNA base pair cocrystals and polynucleotides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 200, 195-201.	3.9	14
56	Structures and properties of large supramolecular coordination complexes predicted with the generalized energy-based fragmentation method. Physical Chemistry Chemical Physics, 2018, 20, 28894-28902.	2.8	8
57	Selective Câ˜N Borylation of Alkyl Amines Promoted by Lewis Base. Angewandte Chemie, 2018, 130, 15447-15451.	2.0	42
58	Selective Câ˜N Borylation of Alkyl Amines Promoted by Lewis Base. Angewandte Chemie - International Edition, 2018, 57, 15227-15231.	13.8	166
59	Biofumigation with volatile organic compounds from Streptomyces alboflavus TDâ€1 and pure chemicals to control Aspergillus ochraceus. Annals of Applied Biology, 2018, 173, 313-322.	2.5	17
60	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. Journal of Chemical Theory and Computation, 2018, 14, 5787-5796.	5.3	21
61	A selenium-catalysed para-amination of phenols. Nature Communications, 2018, 9, 4293.	12.8	43
62	Organocatalytic decarboxylative alkylation of N-hydroxy-phthalimide esters enabled by pyridine-boryl radicals. Chemical Communications, 2018, 54, 11534-11537.	4.1	42
63	â€œInverseâ€•Frustrated Lewis Pairs: An Inverse FLP Approach to the Catalytic Metal Free Hydrogenation of Ketones. Chemistry - A European Journal, 2018, 24, 16526-16531.	3.3	23
64	Fast quantum chemistry calculations for large molecules and condensed-phase systems: The developments and applications of generalized energy-based fragmentation approach. Chinese Science Bulletin, 2018, 63, 3427-3441.	0.7	5
65	Circularly polarized luminescence based chirality transfer of the chiral BINOL moiety via rigid Ï€-conjugation chain backbone structures. Polymer Chemistry, 2017, 8, 1555-1561.	3.9	45
66	Generalized energyâ€based fragmentation approach for modeling condensed phase systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1297.	14.6	38
67	Charge-Transfer-Induced para-Selective sp² Câ€“H Bond Activation of Arenes by Use of a Hypervalent Iodine Compound: A Theoretical Study. Journal of Organic Chemistry, 2017, 82, 2984-2991.	3.2	23
68	Metal-Free Synthesis of C-4 Substituted Pyridine Derivatives Using Pyridine-boryl Radicals via a Radical Addition/Coupling Mechanism: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2017, 139, 3904-3910.	13.7	108
69	Automatic Reaction Pathway Search via Combined Molecular Dynamics and Coordinate Driving Method. Journal of Physical Chemistry A, 2017, 121, 1351-1361.	2.5	61
70	Terahertz spectra of DNA nucleobase crystals: A joint experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 179, 255-260.	3.9	31
71	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 2696-2704.	5.3	34
72	Accurate Relative Energies and Binding Energies of Large Iceâ€“Liquid Water Clusters and Periodic Structures. Journal of Physical Chemistry A, 2017, 121, 4030-4038.	2.5	17

#	Article	IF	Citations
73	Molecular Mechanism of Self-Assembly of Aromatic Oligoamides into Interlocked Double-Helix Foldamers. Journal of Physical Chemistry B, 2017, 121, 10064-10072.	2.6	11
74	Supramolecular catalysis in the methylation of meta-phenylene ethynylene foldamer containing N,N-dimethylaminopyridine. RSC Advances, 2017, 7, 14046-14052.	3.6	3
75	Understanding the polymorphism-dependent emission properties of molecular crystals using a refined QM/MM approach. Physical Chemistry Chemical Physics, 2017, 19, 17516-17520.	2.8	8
76	Rh(<scp>iii</scp>)-catalyzed double Câ€“H activation of aldehyde hydrazones: a route for functionalized 1H-indazole synthesis. Chemical Science, 2017, 8, 1303-1308.	7.4	45
77	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. Journal of Chemical Theory and Computation, 2017, 13, 5231-5239.	5.3	28
78	Multireference Perturbation Theory and Multireference Coupled Cluster Theory Based on the "Block-Correlation" Framework. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2017, 33, 1277-1287.	4.9	3
79	To bridge or not to bridge: The role of sulfuric acid in the Beckmann rearrangement. Chemical Physics Letters, 2016, 659, 100-104.	2.6	5
80	Visibleâ€Light Photoredoxâ€Catalyzed Câ€“H Difluoroalkylation of Hydrazones through an Aminyl Radical/Polar Mechanism. Angewandte Chemie - International Edition, 2016, 55, 2939-2943.	13.8	176
81	Study on THz spectroscopic characteristic of four DNA nucleobases. , 2016, , .		1
82	â€œInverseâ€•Frustrated Lewis Pairs â€“ Activation of Dihydrogen with Organosuperbases and Moderate to Weak Lewis Acids. Journal of the American Chemical Society, 2016, 138, 3286-3289.	13.7	73
83	Finely tuning MOFs towards high performance in C₂H₂ storage: synthesis and properties of a new MOF-505 analogue with an inserted amide functional group. Chemical Communications, 2016, 52, 7241-7244.	4.1	131
84	Vibrational Spectra of Molecular Crystals with the Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2016, 120, 2700-2711.	2.5	27
85	A bipolar macrospirocyclic oligomer based on triphenylamine and 4,5-diazafluorene as a solution-processable host for blue phosphorescent organic light-emitting diodes. Dyes and Pigments, 2016, 134, 348-357.	3.7	13
86	Regulating Circularly Polarized Luminescence Signals of Chiral Binaphthyl-Based Conjugated Polymers by Tuning Dihedral Angles of Binaphthyl Moieties. Macromolecules, 2016, 49, 5444-5451.	4.8	86
87	Circularly Polarized Luminescence of Chiral Perylene Diimide Based Enantiomers Triggered by Supramolecular Selfâ€Assembly. Chemistry - A European Journal, 2016, 22, 12910-12915.	3.3	21
88	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. Journal of Physical Chemistry A, 2016, 120, 9667-9677.	2.5	28
89	Homolytic Cleavage of a Bâ€“B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. Angewandte Chemie - International Edition, 2016, 55, 5985-5989.	13.8	143
90	Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?. Physical Chemistry Chemical Physics, 2016, 18, 16491-16500.	2.8	20

#	Article	IF	Citations
91	Sunlight-promoted cyclization versus decarboxylation in the reaction of alkynoates with N-iodosuccinimide: easy access to 3-iodocoumarins. Green Chemistry, 2016, 18, 3935-3939.	9.0	74
92	Homolytic Cleavage of a Bâ”B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. Angewandte Chemie, 2016, 128, 6089-6093.	2.0	35
93	Hantzsch Ester as a Photosensitizer for the Visibleâ€Lightâ€Induced Debromination of Vicinal Dibromo Compounds. Chemistry - A European Journal, 2016, 22, 9546-9550.	3.3	60
94	Cluster-in-molecule local correlation method for post-Hartreeâ€“Fock calculations of large systems. Molecular Physics, 2016, 114, 1447-1460.	1.7	50
95	Ab initio molecular dynamics with intramolecular noncovalent interactions for unsolvated polypeptides. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
96	The externally corrected coupled cluster approach with four- and five-body clusters from the CASSCF wave function. Journal of Chemical Physics, 2015, 142, 094119.	3.0	8
97	Macrospirocyclic Oligomer Based on Triphenylamine and Diphenylphosphine Oxide as a Bipolar Host for Efficient Blue Electrophosphorescent Organic Light-Emitting Diodes (OLEDs). Organic Letters, 2015, 17, 1413-1416.	4.6	25
98	Tuning Charge Balance in Solution-Processable Bipolar Triphenylamine-diazafluorene Host Materials for Phosphorescent Devices. ACS Applied Materials & Interfaces, 2015, 7, 9445-9452.	8.0	17
99	Mechanistic insights into the full hydrogenation of 2,6-substituted pyridine catalyzed by the Lewis acid C₆F₅(CH₂)₂B(C₆F₅)₂. Dalton Transactions, 2015, 44, 9200-9208.	3.3	15
100	Understanding the Boronâ€“Nitrogen Interaction and Its Possible Implications in Drug Design. Journal of Physical Chemistry B, 2015, 119, 14393-14401.	2.6	5
101	An insight into the Lewis acid-catalyzed intramolecular aminocyanation and oxycyanation of alkenes: a concerted or stepwise mechanism. Chemical Communications, 2015, 51, 15450-15453.	4.1	11
102	Multireference Second Order Perturbation Theory with a Simplified Treatment of Dynamical Correlation. Journal of Chemical Theory and Computation, 2015, 11, 4634-4643.	5.3	20
103	LSQC: Low scaling quantum chemistry program. International Journal of Quantum Chemistry, 2015, 115, 641-646.	2.0	57
104	Accurate Prediction of Lattice Energies and Structures of Molecular Crystals with Molecular Quantum Chemistry Methods. Journal of Chemical Theory and Computation, 2015, 11, 91-98.	5.3	45
105	The relative energies of polypeptide conformers predicted by linear scaling second-order MÃ¸ller-Plesset perturbation theory. Science China Chemistry, 2014, 57, 1393-1398.	8.2	12
106	An efficient localization procedure for large systems using a sequential transformation strategy. Journal of Chemical Physics, 2014, 141, 244106.	3.0	12
107	Structural preferences of two unnatural hybrid octapeptides with and without the crystal environment: a computational study. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	1
108	Efficient Implementation of Local Excitation Approximation for Treating Excited States of Molecules in Condensed Phase. Journal of Chemical Theory and Computation, 2014, 10, 5308-5317.	5.3	7

#	Article	IF	Citations
109	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. Accounts of Chemical Research, 2014, 47, 2712-2720.	15.6	143
110	Cluster-in-molecule local correlation method for large systems. Science China Chemistry, 2014, 57, 78-86.	8.2	20
111	Improved Cluster-in-Molecule Local Correlation Approach for Electron Correlation Calculation of Large Systems. Journal of Physical Chemistry A, 2014, 118, 8996-9004.	2.5	40
112	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H₂O)₂₀. Journal of Chemical Theory and Computation, 2014, 10, 1546-1553.	5.3	62
113	The Generalized Energyâ€Based Fragmentation Approach with an Improved Fragmentation Scheme: Benchmark Results and Illustrative Applications. ChemPhysChem, 2013, 14, 108-115.	2.1	35
114	Mechanistic Insight on the Dielsâ€“Alder Reaction Catalyzed by a Self-Assembled Molecular Capsule. Journal of Organic Chemistry, 2013, 78, 3577-3582.	3.2	20
115	Insight into the reaction between a primary amine and a cavitand with an introverted aldehyde group: an enzyme-like mechanism. Chemical Communications, 2013, 49, 1542.	4.1	23
116	Hybrid Coupled Cluster Methods Based on the Split Virtual Orbitals: Barrier Heights of Reactions and Spectroscopic Constants of Open-Shell Diatomic Molecules. Journal of Physical Chemistry A, 2013, 117, 626-632.	2.5	2
117	Block correlated second order perturbation theory with a generalized valence bond reference function. Journal of Chemical Physics, 2013, 139, 174111.	3.0	40
118	The coupled cluster singles, doubles, and a hybrid treatment of connected triples based on the split virtual orbitals. Journal of Chemical Physics, 2012, 136, 044101.	3.0	3
119	Hybrid coupled cluster methods: Combining active space coupled cluster methods with coupled cluster singles, doubles, and perturbative triples. Journal of Chemical Physics, 2012, 136, 194105.	3.0	6
120	A refined cluster-in-molecule local correlation approach for predicting the relative energies of large systems. Physical Chemistry Chemical Physics, 2012, 14, 7854.	2.8	50
121	High and selective CO2 capture by two mesoporous acylamide-functionalized rht-type metalâ€“organic frameworks. Chemical Communications, 2012, 48, 7025.	4.1	174
122	An improved localized molecular-orbital assembler approach for Hartreeâ€–Fock calculations of general large molecules. Chemical Physics Letters, 2012, 539-540, 186-190.	2.6	5
123	Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes. Chemical Physics Letters, 2012, 541, 7-11.	2.6	20
124	Highly selective CO2 capture of an agw-type metalâ€“organic framework with inserted amides: experimental and theoretical studies. Chemical Communications, 2012, 48, 3058.	4.1	166
125	The coupled cluster approach with a hybrid treatment of connected triple excitations: Spectroscopic constants in open-shell diatomic molecules, and bond-breaking or twisting potential energy surfaces. Chemical Physics, 2012, 401, 113-118.	1.9	4
126	Experimental and theoretical magneto-structural studies on the dicarboxylato-bridged nature of the dicopper(II)-based metalâ€“organic frameworks. Inorganica Chimica Acta, 2012, 387, 137-144.	2.4	7

#	Article	IF	Citations
127	New Insights into the Molecular Mechanism of H2 Activation. , 2012, , 47-60.		0
128	Structures of Neutral and Protonated Water Clusters Confined in Predesigned Hosts: A Quantum Mechanical/Molecular Mechanical Study. Journal of Physical Chemistry B, 2011, 115, 8249-8256.	2.6	13
129	New coupled cluster approaches based on the unrestricted Hartreeâ€“Fock reference for treating molecules with multireference character. Physical Chemistry Chemical Physics, 2011, 13, 8795.	2.8	16
130	Cooperativity in Long Î±- and 3₁₀-Helical Polyalanines: Both Electrostatic and van der Waals Interactions Are Essential. Journal of Physical Chemistry B, 2011, 115, 11462-11469.	2.6	35
131	A coupled cluster approach with excitations up to six orbital pairs: The formulation and test applications for bond breaking processes. Journal of Chemical Physics, 2011, 134, 234104.	3.0	3
132	Insights into Dehydrogenative Coupling of Alcohols and Amines Catalyzed by a (PNN)â€“Ru(II) Hydride Complex: Unusual Metalâ€“Ligand Cooperation. Inorganic Chemistry, 2011, 50, 10572-10580.	4.0	72
133	Understanding the Influence of Guestâ€“Host Interactions on the Conformation of Short Peptides in a Hydrophobic Cavity: A Computational Study. ChemPhysChem, 2011, 12, 1325-1333.	2.1	2
134	The coupled cluster approach with a hybrid treatment of connected triple excitations based on the restricted Hartreeâ€“Fock reference. Journal of Chemical Physics, 2011, 134, 044134.	3.0	15
135	An efficient linear scaling procedure for constructing localized orbitals of large molecules based on the one-particle density matrix. Journal of Chemical Physics, 2011, 135, 134107.	3.0	17
136	A coupled cluster approach with a hybrid treatment of connected triple excitations: Implementation and applications for open-shell systems. Journal of Chemical Physics, 2010, 133, 234106.	3.0	15
137	X-ray absorption spectra of graphene from first-principles simulations. Physical Review B, 2010, 82, .	3.2	78
138	Comparison of some multireference electronic structure methods in illustrative applications. Science China Chemistry, 2010, 53, 289-296.	8.2	1
139	Theoretical Study on the Mechanism of the Petasisâ€type Boronic Mannich Reaction of Organoboronic Acids, Amines, and Î±â€Hydroxy Aldehydes. Chinese Journal of Chemistry, 2010, 28, 41-49.	4.9	22
140	A coupled cluster approach with a hybrid treatment of connected triple excitations for bond-breaking potential energy surfaces. Journal of Chemical Physics, 2010, 132, 114115.	3.0	22
141	Coupled cluster with singles, doubles, and partial higher-order excitations based on the corresponding orbitals: The formulation and test applications for bond breaking processes. Journal of Chemical Physics, 2010, 132, 134110.	3.0	12
142	Block Correlated Coupled Cluster Theory With A Complete Active-Space Self-Consistent-Field Reference Function: The General Formalism And Applications. Challenges and Advances in Computational Chemistry and Physics, 2010, , 145-174.	0.6	3
143	An Efficient Implementation of the Generalized Energy-Based Fragmentation Approach for General Large Molecules. Journal of Physical Chemistry A, 2010, 114, 8126-8134.	2.5	91
144	Refinement of DNA Structures through Near-Edge X-ray Absorption Fine Structure Analysis: Applications on Guanine and Cytosine Nucleobases, Nucleosides, and Nucleotides. Journal of Physical Chemistry B, 2010, 114, 13214-13222.	2.6	25

#	Article	IF	Citations
145	Systematic Study of Soft X-ray Spectra of Poly(Dg)Â·Poly(Dc) and Poly(Da)Â·Poly(Dt) DNA Duplexes. Journal of Physical Chemistry B, 2010, 114, 7016-7021.	2.6	24
146	Mechanistic Insight on the Hydrogenation of Conjugated Alkenes with H2Catalyzed by Early Main-Group Metal Catalysts. Inorganic Chemistry, 2010, 49, 3361-3369.	4.0	33
147	Low-Lying Structures and Stabilities of Large Water Clusters: Investigation Based on the Combination of the AMOEBA Potential and Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2010, 114, 9253-9261.	2.5	43
148	Theoretical study on the mechanism of H₂activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh. Dalton Transactions, 2010, 39, 857-863.	3.3	21
149	Stress influence on band-edge luminescence properties of 4H-AlN. Applied Physics Letters, 2009, 95, 121902.	3.3	2
150	Block correlated coupled cluster method with the complete active-space self-consistent-field reference function: Applications for low-lying electronic excited states. Journal of Chemical Physics, 2009, 131, 174101.	3.0	27
151	Local correlation calculations using standard and renormalized coupled-cluster approaches. Journal of Chemical Physics, 2009, 131, 114109.	3.0	199
152	Interpretation of the characteristic fragmentation mechanisms through determining the initial ionization site by natural spin density: A study on the derivatives of tryptophan and tryptamine. International Journal of Mass Spectrometry, 2009, 286, 112-121.	1.5	11
153	Understanding the role of the bifunctional titanium catalyst in cyanosilylation of ketones: A computational study. Computational and Theoretical Chemistry, 2009, 899, 61-70.	1.5	6
154	H2 Activation by a (PNP)Ir(C6H5) Complex via the Dearomatization/Aromatization Process of the PNP Ligand: A Computational Study. Inorganic Chemistry, 2009, 48, 10257-10263.	4.0	43
155	Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 1335-1342.	2.5	24
156	Optical and vibrational properties of 2H-, 4H-, and 6H-AlN: First-principle calculations. Journal of Applied Physics, 2009, 105, 083511.	2.5	11
157	Raman scattering study of zinc blende and wurtzite ZnS. Journal of Applied Physics, 2009, 106, .	2.5	235
158	Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for Carbonâ€“Carbon Bond Breaking in Hydrocarbons. Progress in Theoretical Chemistry and Physics, 2009, , 241-255.	0.2	1
159	Singlet-triplet gaps in substituted carbenes predicted from block-correlated coupled cluster method. Science in China Series B: Chemistry, 2008, 51, 1197-1202.	0.8	6
160	A Novel Addition Mechanism for the Reaction of â€œFrustrated Lewis Pairsâ€•with Olefins. European Journal of Inorganic Chemistry, 2008, 2008, 2501-2505.	2.0	85
161	Energetics and Mechanism of Dinitrogen Cleavage at a Mononuclear Surface Tantalum Center: A New Way of Dinitrogen Reduction. Angewandte Chemie - International Edition, 2008, 47, 8040-8043.	13.8	27
162	Ab initio determination of lattice dynamics and thermodynamics of Î² - BC2N. Solid State Communications, 2008, 146, 69-72.	1.9	11

#	Article	IF	Citations
163	Fragment energy approach to Hartreeâ€“Fock calculations of macromolecules. Annual Reports on the Progress of Chemistry Section C, 2008, 104, 256.	4.4	22
164	Unusual Concerted Lewis Acidâ€'Lewis Base Mechanism for Hydrogen Activation by a Phosphineâ€'Borane Compound. Inorganic Chemistry, 2008, 47, 6212-6219.	4.0	123
165	Optical properties of rocksalt and zinc blende AlN phases: First-principles calculations. Journal of Applied Physics, 2008, 103, .	2.5	61
166	Metal-Induced Bâ€'H Bond Activation: Addition of Methyl Acetylene Monocarboxylate to CpCo Half-Sandwich Complexes Containing a Chelating 1,2-Dicarba-closo-dodecaborane-1,2-dichalcogenolate Ligand. Organometallics, 2008, 27, 334-340.	2.3	46
167	Temperature Controlled Reversible Change of the Coordination Modes of the Highly Symmetrical Multitopic Ligand To Construct Coordination Assemblies: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2008, 130, 7778-7779.	13.7	254
168	Fragmentation-Based QM/MM Simulations: Length Dependence of Chain Dynamics and Hydrogen Bonding of Polyethylene Oxide and Polyethylene in Aqueous Solutions. Journal of Physical Chemistry B, 2008, 112, 7061-7070.	2.6	31
169	Spectroscopic Constants of Single-Bond Diatomic Molecules and Singletâ€'Triplet Gaps of Diradicals by the Block-Correlated Coupled Cluster Theory. Journal of Physical Chemistry A, 2008, 112, 4703-4709.	2.5	24
170	Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for the Prediction of Activation Barriers, Spectroscopic Constants in Diatomic Molecules, and Singletâ€'Triplet Gaps in Diradicals. Journal of Physical Chemistry A, 2008, 112, 12518-12525.	2.5	29
171	A DFT Study toward Understanding the High Activity of Fe-Exchanged Zeolites for the â€œFastâ€•Selective Catalytic Reduction of Nitrogen Oxides with Ammonia. Journal of Physical Chemistry C, 2008, 112, 16938-16944.	3.1	50
172	Geometry Optimizations and Vibrational Spectra of Large Molecules from a Generalized Energy-Based Fragmentation Approach. Journal of Physical Chemistry A, 2008, 112, 10864-10872.	2.5	121
173	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The implementation for low-lying excited states. Journal of Chemical Physics, 2008, 129, 234106.	3.0	16
174	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The formula for general active spaces and its applications for multibond breaking systems. Journal of Chemical Physics, 2008, 128, 224107.	3.0	41
175	Relative Energies of Proteins and Water Clusters Predicted with the Generalized Energy-Based Fragmentation Approach. Progress in Theoretical Chemistry and Physics, 2008, , 289-299.	0.2	3
176	Block correlated coupled cluster theory with a complete active-space self-consistent-field reference function: The formulation and test applications for single bond breaking. Journal of Chemical Physics, 2007, 127, 204108.	3.0	54
177	Interfacial Charge Transfer and Transport in Polyacetylene-Based Heteroionic Junctions:Â Quantum Chemistry Calculations and Molecular Dynamics Simulations. Macromolecules, 2007, 40, 4363-4369.	4.8	14
178	Metal complexes formed by metal-assisted solvolysis of di-pyridylketone azine: structures and magnetic properties. Dalton Transactions, 2007, , 1838.	3.3	21
179	New insight into selective catalytic reduction of nitrogen oxides by ammonia over H-form zeolites: a theoretical study. Physical Chemistry Chemical Physics, 2007, 9, 3304.	2.8	27
180	Estimation on the Individual Hydrogen-Bond Strength in Molecules with Multiple Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 2941-2945.	2.5	52

#	Article	IF	Citations
181	Generalized Energy-Based Fragmentation Approach for Computing the Ground-State Energies and Properties of Large Molecules. Journal of Physical Chemistry A, 2007, 111, 2193-2199.	2.5	254
182	A Smart Supramolecular Hydrogel Exhibiting pH-Modulated Viscoelastic Properties. Advanced Functional Materials, 2007, 17, 1837-1843.	14.9	91
183	Tetranuclear manganese(III) clusters containing both carboxylate and phosphonate bridging ligands. Inorganica Chimica Acta, 2007, 360, 1645-1650.	2.4	36
184	A Large Protonated Water Cluster H+(H2O)27in a 3D Metalâ^'Organic Framework. Journal of the American Chemical Society, 2006, 128, 13318-13319.	13.7	218
185	A supramolecular assembly of {Fe10} molecular wheels with tubular structures. CrystEngComm, 2006, 8, 384.	2.6	13
186	Theoretical Study on the Excitation Energies of Six Tautomers of Guanine:Â Evidence for the Assignment of the Rare Tautomers. Journal of Physical Chemistry A, 2006, 110, 12360-12362.	2.5	53
187	Catalytic Mechanism of 6-Phosphogluconate Dehydrogenase:Â A Theoretical Investigation. Journal of Physical Chemistry B, 2006, 110, 7029-7035.	2.6	6
188	Theoretical Study on the Dielsâ^'Alder Reaction between 2-Methylacrolein and Cyclopentadiene Catalyzed by a Cationic Oxazaborolidine Lewis Acid. Journal of Physical Chemistry A, 2006, 110, 9225-9230.	2.5	16
189	CASPT2//CASSCF Study on the Photolysis Mechanism of 2,3-Diazabicyclo[2.1.1]hex-2-ene:â€‰ Î± Câ^'N versus Î² Câ^'C Cleavage. Journal of Organic Chemistry, 2006, 71, 9013-9022.	3.2	6
190	A multireference configuration interaction method based on the separated electron pair wave functions. Journal of Computational Chemistry, 2006, 27, 39-47.	3.3	28
191	An efficient implementation of the â€œcluster-in-moleculeâ€•approach for local electron correlation calculations. Journal of Chemical Physics, 2006, 125, 074109.	3.0	126
192	Ab initiostudy on deactivation pathways of excited 9H-guanine. Journal of Chemical Physics, 2006, 124, 154315.	3.0	93
193	A fragment energy assembler method for Hartree-Fock calculations of large molecules. Journal of Chemical Physics, 2006, 124, 154102.	3.0	39
194	THEORETICAL STUDY TOWARD UNDERSTANDING THE CATALYTIC MECHANISM OF PYRUVATE DEHYDROGENASE MULTIENZYME COMPLEX E1 COMPONENT. Journal of Theoretical and Computational Chemistry, 2006, 05, 447-459.	1.8	3
195	A localized molecular-orbital assembler approach for Hartreeâ€“Fock calculations of large molecules. Journal of Chemical Physics, 2005, 122, 194109.	3.0	45
196	Theoretical Study toward Understanding Ultrafast Internal Conversion of Excited 9H-Adenine. Journal of Physical Chemistry A, 2005, 109, 8443-8446.	2.5	87
197	Theoretical Study on the Photolysis Mechanism of 2,3-Diazabicyclo[2.2.2]oct-2-ene. Journal of the American Chemical Society, 2005, 127, 13190-13199.	13.7	5
198	A Theoretical Study of the Mechanism of Phosphine-Catalyzed Hydroalkoxylation of Methyl Vinyl Ketone. Journal of Physical Chemistry A, 2005, 109, 10770-10775.	2.5	13

#	Article	IF	Citations
199	Mechanism of Ruthenium-Catalyzed Alder Ene-Type Reaction:â€‰ A Theoretical Study. Organometallics, 2005, 24, 872-884.	2.3	14
200	An Efficient Fragment-Based Approach for Predicting the Ground-State Energies and Structures of Large Molecules. Journal of the American Chemical Society, 2005, 127, 7215-7226.	13.7	208
201	Theoretical Study toward Understanding the Catalytic Mechanism of Pyruvate Decarboxylase. Journal of Physical Chemistry B, 2005, 109, 18664-18672.	2.6	30
202	Block-correlated coupled cluster theory:â€‰The general formulation and its application to the antiferromagnetic Heisenberg model. Journal of Chemical Physics, 2004, 120, 5017-5026.	3.0	61
203	Divide-and-conquer local correlation approach to the correlation energy of large molecules. Journal of Chemical Physics, 2004, 121, 6649-6657.	3.0	95
204	Mechanism of H2O2Dismutation Catalyzed by a New Catalase Mimic (a Non-Heme) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 Td (Diber Chemistry, 2004, 43, 6479-6489.	4.0	13
205	Density Functional Study on the Mechanisms of the Reactions of Gas-Phase OsOn+ (n = 1â˜’4) with Methane. Organometallics, 2004, 23, 3656-3667.	2.3	27
206	Substituent effect of the spin-coupling constant through m-phenylene in m-xylylene and its derivatives. Tetrahedron, 2003, 59, 3499-3504.	1.9	10
207	Dehydrogenation of Methane by Gas-Phase Os+:Â A Density Functional Study. Organometallics, 2003, 22, 3820-3830.	2.3	57
208	A Density Functional Theory Study on the Intramolecular Proton Transfer in the Enzyme Carbonic Anhydrase. Journal of Physical Chemistry A, 2003, 107, 4652-4660.	2.5	13
209	Effects of Substitution on the Singletâ˜’Triplet Energy Splittings and Ground-State Multiplicities of m-Phenylene-Based Diradicals:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry A, 2003, 107, 5573-5582.	2.5	45
210	Pair-correlated coupled cluster theory: An alternative multireference coupled cluster method. Journal of Chemical Physics, 2003, 118, 5736-5745.	3.0	23
211	The Valence Bond Calculations on Conjugated Hydrocarbons of Medium to Infinite Sizes. Journal of the Chinese Chemical Society, 2003, 50, 717-728.	1.4	1
212	A Quick Estimate of the Correlation Energy for Alkanes. Chinese Journal of Chemistry, 2003, 21, 1422-1429.	4.9	15
213	HEISENBERG MODEL AND ITS APPLICATIONS TO Ï€-CONJUGATED SYSTEMS. Journal of Theoretical and Computational Chemistry, 2002, 01, 351-371.	1.8	3
214	A Time-Dependent DFT Study on Band Gaps and Effective Conjugation Lengths of Polyacetylene, Polyphenylene, Polypentafulvene, Polycyclopentadiene, Polypyrrole, Polyfuran, Polysilole, Polyphosphole, and Polythiophene. Macromolecules, 2002, 35, 1109-1115.	4.8	205
215	Linear scaling local correlation approach for solving the coupled cluster equations of large systems. Journal of Computational Chemistry, 2002, 23, 237-244.	3.3	181
216	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of Desulfovibrio fructosovorans Ni-Fe hydrogenase. Journal of Biological Inorganic Chemistry, 2002, 7, 318-326.	2.6	78

#	Article	IF	Citations
217	An MP2 study of linear polarizabilities and second-order hyperpolarizabilities for centrosymmetric squaraines. Chemical Physics Letters, 2002, 354, 316-323.	2.6	22
218	KekulÃ©â€based Valence Bond Model. I. The Groundâ€state Properties of Conjugated 7Ã¼â€Systems. Chinese Journal of Chemistry, 2002, 20, 1168-1179.	4.9	4
219	KekulÃ©â€based Valence Bond Model. II. Dielsâ€Alder Reactivity of Polycyclic Aromatic Hydrocarbons. Chinese Journal of Chemistry, 2002, 20, 1180-1191.	4.9	1
220	Modeling the Active Sites of Metalloenzymes. 4. Predictions of the Unready States of [NiFe]Desulfovibrio gigasHydrogenase from Density Functional Theory. Inorganic Chemistry, 2001, 40, 18-24.	4.0	61
221	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 18. Catalytic Transfer Dehydrogenation of Alkanes by an Iridium(III) Pincer Complex. Organometallics, 2001, 20, 2153-2160.	2.3	38
222	Pair-correlated configuration interaction method and its approximate version for solving the electron correlation problem in molecules. International Journal of Quantum Chemistry, 2000, 78, 153-167.	2.0	6
223	Transition Metal Polyhydride Complexes. 10. Intramolecular Hydrogen Exchange in the Octahedral Iridium(III) Dihydrogen Dihydride Complexes IrXH2(Î·2-H2)(PR3)2(X = Cl, Br, I). Journal of the American Chemical Society, 2000, 122, 2903-2910.	13.7	38
224	Transition Metal Polyhydride Complexes. 11. Mechanistic Studies of the Cis to Trans Isomerization of the Iridium(III) Dihydride Ir(H)2(CO)L (L = C6H3(CH2P(H)2)2). Organometallics, 1999, 18, 5682-5687.	2.3	26
225	Can the Low-Lying Electronic States of Benzenoid Hydrocarbons Be Described by the Semiempirical Valence Bond Approach?. Journal of Physical Chemistry A, 1997, 101, 4770-4775.	2.5	8
226	Strength of Spin Coupling in High-Spin Organic Molecules. Journal of Physical Chemistry A, 1997, 101, 5567-5573.	2.5	33
227	Electron Correlation and Magnetism:Â A Simple Molecular Orbital Approach for Predicting Ground-State Spins of Conjugated Hydrocarbons. Journal of Physical Chemistry A, 1997, 101, 5587-5592.	2.5	17
228	Is Ferromagnetic Spin Coupling Constant within Homologous Di- and Triradicals?. The Journal of Physical Chemistry, 1996, 100, 4775-4780.	2.9	28
229	Effective Valence Bond Model Study on Conjugated Hydrocarbons Containing Four-Membered Rings. The Journal of Physical Chemistry, 1996, 100, 15068-15072.	2.9	12
230	The Hubbard transition in molecular systems. Chemical Physics Letters, 1995, 241, 57-61.	2.6	2
231	Topological dependence of ferromagnetic coupling strength in some Ï€-conjugated radicals. Chemical Physics Letters, 1995, 246, 221-227.	2.6	12
232	Bond Lengths, Reactivities, and Aromaticities of Benzenoid Hydrocarbons Based on Valence Bond Calculations. Journal of the American Chemical Society, 1995, 117, 8401-8406.	13.7	39