

Shu-Hua Li

List of Publications by Year in descending order

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232
papers

8,916
citations

41258

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248
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248
times ranked

7655
citing authors

#	ARTICLE	IF	CITATIONS
1	Generalized Energy-Based Fragmentation Approach for Computing the Ground-State Energies and Properties of Large Molecules. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2193-2199.	1.1	254
2	Temperature Controlled Reversible Change of the Coordination Modes of the Highly Symmetrical Multitopic Ligand To Construct Coordination Assemblies: Experimental and Theoretical Studies. <i>Journal of the American Chemical Society</i> , 2008, 130, 7778-7779.	6.6	254
3	Targeted tumour theranostics in mice via carbon quantum dots structurally mimicking large amino acids. <i>Nature Biomedical Engineering</i> , 2020, 4, 704-716.	11.6	243
4	Raman scattering study of zinc blende and wurtzite ZnS. <i>Journal of Applied Physics</i> , 2009, 106, .	1.1	235
5	A Large Protonated Water Cluster H ⁺ (H ₂ O) ₂₇ in a 3D Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2006, 128, 13318-13319.	6.6	218
6	An Efficient Fragment-Based Approach for Predicting the Ground-State Energies and Structures of Large Molecules. <i>Journal of the American Chemical Society</i> , 2005, 127, 7215-7226.	6.6	208
7	A Time-Dependent DFT Study on Band Gaps and Effective Conjugation Lengths of Polyacetylene, Polyphenylene, Polypentafulvene, Polycyclopentadiene, Polypyrrole, Polyfuran, Polysilole, Polyphosphole, and Polythiophene. <i>Macromolecules</i> , 2002, 35, 1109-1115.	2.2	205
8	Local correlation calculations using standard and renormalized coupled-cluster approaches. <i>Journal of Chemical Physics</i> , 2009, 131, 114109.	1.2	199
9	Linear scaling local correlation approach for solving the coupled cluster equations of large systems. <i>Journal of Computational Chemistry</i> , 2002, 23, 237-244.	1.5	181
10	Visible-Light Photoredox-Catalyzed C-H Difluoroalkylation of Hydrazones through an Aminyl Radical/Polar Mechanism. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2939-2943.	7.2	176
11	High and selective CO ₂ capture by two mesoporous acylamide-functionalized rht-type metal-organic frameworks. <i>Chemical Communications</i> , 2012, 48, 7025.	2.2	174
12	Highly selective CO ₂ capture of an agw-type metal-organic framework with inserted amides: experimental and theoretical studies. <i>Chemical Communications</i> , 2012, 48, 3058.	2.2	166
13	Selective C-N Borylation of Alkyl Amines Promoted by Lewis Base. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15227-15231.	7.2	166
14	Generalized Energy-Based Fragmentation Approach and Its Applications to Macromolecules and Molecular Aggregates. <i>Accounts of Chemical Research</i> , 2014, 47, 2712-2720.	7.6	143
15	Homolytic Cleavage of a B-B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5985-5989.	7.2	143
16	Finely tuning MOFs towards high performance in C ₂ H ₂ storage: synthesis and properties of a new MOF-505 analogue with an inserted amide functional group. <i>Chemical Communications</i> , 2016, 52, 7241-7244.	2.2	131
17	An efficient implementation of the ϵ -cluster-in-molecule approach for local electron correlation calculations. <i>Journal of Chemical Physics</i> , 2006, 125, 074109.	1.2	126
18	Unusual Concerted Lewis Acid-Lewis Base Mechanism for Hydrogen Activation by a Phosphine-Borane Compound. <i>Inorganic Chemistry</i> , 2008, 47, 6212-6219.	1.9	123

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19	Geometry Optimizations and Vibrational Spectra of Large Molecules from a Generalized Energy-Based Fragmentation Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10864-10872.	1.1	121
20	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. <i>Journal of the American Chemical Society</i> , 2017, 139, 3904-3910.	6.6	108
21	Cooperative Au/Ag Dual-Catalyzed Cross-Dehydrogenative Biaryl Coupling: Reaction Development and Mechanistic Insight. <i>Journal of the American Chemical Society</i> , 2019, 141, 3187-3197.	6.6	101
22	Divide-and-conquer local correlation approach to the correlation energy of large molecules. <i>Journal of Chemical Physics</i> , 2004, 121, 6649-6657.	1.2	95
23	Ab initio study on deactivation pathways of excited 9H-guanine. <i>Journal of Chemical Physics</i> , 2006, 124, 154315.	1.2	93
24	A Smart Supramolecular Hydrogel Exhibiting pH-Modulated Viscoelastic Properties. <i>Advanced Functional Materials</i> , 2007, 17, 1837-1843.	7.8	91
25	An Efficient Implementation of the Generalized Energy-Based Fragmentation Approach for General Large Molecules. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8126-8134.	1.1	91
26	Theoretical Study toward Understanding Ultrafast Internal Conversion of Excited 9H-Adenine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8443-8446.	1.1	87
27	Regulating Circularly Polarized Luminescence Signals of Chiral Binaphthyl-Based Conjugated Polymers by Tuning Dihedral Angles of Binaphthyl Moieties. <i>Macromolecules</i> , 2016, 49, 5444-5451.	2.2	86
28	A Novel Addition Mechanism for the Reaction of σ -Frustrated Lewis Pairs with Olefins. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2501-2505.	1.0	85
29	Perfluoroalkylative pyridylation of alkenes via 4-cyanopyridine-boryl radicals. <i>Chemical Science</i> , 2019, 10, 2767-2772.	3.7	81
30	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of <i>Desulfovibrio fructosovorans</i> Ni-Fe hydrogenase. <i>Journal of Biological Inorganic Chemistry</i> , 2002, 7, 318-326.	1.1	78
31	X-ray absorption spectra of graphene from first-principles simulations. <i>Physical Review B</i> , 2010, 82, .	1.1	78
32	Sunlight-promoted cyclization versus decarboxylation in the reaction of alkynoates with N-iodosuccinimide: easy access to 3-iodocoumarins. <i>Green Chemistry</i> , 2016, 18, 3935-3939.	4.6	74
33	σ -Frustrated Lewis Pairs Activation of Dihydrogen with Organosuperbases and Moderate to Weak Lewis Acids. <i>Journal of the American Chemical Society</i> , 2016, 138, 3286-3289.	6.6	73
34	Insights into Dehydrogenative Coupling of Alcohols and Amines Catalyzed by a (PNN) σ -Ru(II) Hydride Complex: Unusual Metal-Ligand Cooperation. <i>Inorganic Chemistry</i> , 2011, 50, 10572-10580.	1.9	72
35	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H ₂ O) ₂₀ . <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1546-1553.	2.3	62
36	Modeling the Active Sites of Metalloenzymes. 4. Predictions of the Unready States of [NiFe]Desulfovibrio gasHydrogenase from Density Functional Theory. <i>Inorganic Chemistry</i> , 2001, 40, 18-24.	1.9	61

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37	Block-correlated coupled cluster theory: The general formulation and its application to the antiferromagnetic Heisenberg model. <i>Journal of Chemical Physics</i> , 2004, 120, 5017-5026.	1.2	61
38	Optical properties of rocksalt and zinc blende AlN phases: First-principles calculations. <i>Journal of Applied Physics</i> , 2008, 103, .	1.1	61
39	Automatic Reaction Pathway Search via Combined Molecular Dynamics and Coordinate Driving Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1351-1361.	1.1	61
40	Hantzsch Ester as a Photosensitizer for the Visible-Light-Induced Debromination of Vicinal Dibromo Compounds. <i>Chemistry - A European Journal</i> , 2016, 22, 9546-9550.	1.7	60
41	Dehydrogenation of Methane by Gas-Phase Os ⁺ : A Density Functional Study. <i>Organometallics</i> , 2003, 22, 3820-3830.	1.1	57
42	LSQC: Low scaling quantum chemistry program. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 641-646.	1.0	57
43	Organocatalytic reductive coupling of aldehydes with 1,1-diarylethylenes using an <i>in situ</i> generated pyridine-boryl radical. <i>Chemical Science</i> , 2018, 9, 3664-3671.	3.7	56
44	Block correlated coupled cluster theory with a complete active-space self-consistent-field reference function: The formulation and test applications for single bond breaking. <i>Journal of Chemical Physics</i> , 2007, 127, 204108.	1.2	54
45	Chemoselective Borane-Catalyzed Hydroarylation of 1,3-Dienes with Phenols. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 1694-1699.	7.2	54
46	Theoretical Study on the Excitation Energies of Six Tautomers of Guanine: Evidence for the Assignment of the Rare Tautomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12360-12362.	1.1	53
47	Estimation on the Individual Hydrogen-Bond Strength in Molecules with Multiple Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2941-2945.	1.1	52
48	A DFT Study toward Understanding the High Activity of Fe-Exchanged Zeolites for the Fast-Selective Catalytic Reduction of Nitrogen Oxides with Ammonia. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16938-16944.	1.5	50
49	A refined cluster-in-molecule local correlation approach for predicting the relative energies of large systems. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7854.	1.3	50
50	Cluster-in-molecule local correlation method for post-Hartree-Fock calculations of large systems. <i>Molecular Physics</i> , 2016, 114, 1447-1460.	0.8	50
51	Transition-Metal-Free Defluorosilylation of Fluoroalkenes with Silylboronates. <i>Chinese Journal of Chemistry</i> , 2019, 37, 1009-1014.	2.6	49
52	Metal-Induced B-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. <i>Organometallics</i> , 2008, 27, 334-340.	1.1	46
53	Photoredox-Controlled Regioselective Radical Hydroboration of Activated Alkenes with NHC-Boranes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12817-12821.	7.2	46
54	Effects of Substitution on the Singlet-Triplet Energy Splittings and Ground-State Multiplicities of m-Phenylene-Based Diradicals: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5573-5582.	1.1	45

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55	A localized molecular-orbital assembler approach for Hartree-Fock calculations of large molecules. <i>Journal of Chemical Physics</i> , 2005, 122, 194109.	1.2	45
56	Accurate Prediction of Lattice Energies and Structures of Molecular Crystals with Molecular Quantum Chemistry Methods. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 91-98.	2.3	45
57	Circularly polarized luminescence based chirality transfer of the chiral BINOL moiety via rigid π -conjugation chain backbone structures. <i>Polymer Chemistry</i> , 2017, 8, 1555-1561.	1.9	45
58	Rh-catalyzed double C-H activation of aldehyde hydrazones: a route for functionalized 1H-indazole synthesis. <i>Chemical Science</i> , 2017, 8, 1303-1308.	3.7	45
59	H ₂ Activation by a (PNP)Ir(C ₆ H ₅) Complex via the Dearomatization/Aromatization Process of the PNP Ligand: A Computational Study. <i>Inorganic Chemistry</i> , 2009, 48, 10257-10263.	1.9	43
60	Low-Lying Structures and Stabilities of Large Water Clusters: Investigation Based on the Combination of the AMOEBA Potential and Generalized Energy-Based Fragmentation Approach. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9253-9261.	1.1	43
61	A selenium-catalysed para-amination of phenols. <i>Nature Communications</i> , 2018, 9, 4293.	5.8	43
62	Selective C ¹⁵ N Borylation of Alkyl Amines Promoted by Lewis Base. <i>Angewandte Chemie</i> , 2018, 130, 15447-15451.	1.6	42
63	Organocatalytic decarboxylative alkylation of <i>N</i> -hydroxy-phthalimide esters enabled by pyridine-boryl radicals. <i>Chemical Communications</i> , 2018, 54, 11534-11537.	2.2	42
64	Lewis Acid-Catalyzed Selective Reductive Decarboxylative Pyridylation of <i>N</i> -Hydroxyphthalimide Esters: Synthesis of Congested Pyridine-Substituted Quaternary Carbons. <i>ACS Catalysis</i> , 2019, 9, 10142-10151.	5.5	42
65	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. <i>Journal of Chemical Physics</i> , 2008, 128, 224107.	1.2	41
66	Block correlated second order perturbation theory with a generalized valence bond reference function. <i>Journal of Chemical Physics</i> , 2013, 139, 174111.	1.2	40
67	Improved Cluster-in-Molecule Local Correlation Approach for Electron Correlation Calculation of Large Systems. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8996-9004.	1.1	40
68	Bond Lengths, Reactivities, and Aromaticities of Benzenoid Hydrocarbons Based on Valence Bond Calculations. <i>Journal of the American Chemical Society</i> , 1995, 117, 8401-8406.	6.6	39
69	A fragment energy assembler method for Hartree-Fock calculations of large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 154102.	1.2	39
70	Transition Metal Polyhydride Complexes. 10. Intramolecular Hydrogen Exchange in the Octahedral Iridium(III) Dihydrogen Dihydride Complexes IrXH ₂ (η -2-H ₂)(PR ₃) ₂ (X = Cl, Br, I). <i>Journal of the American Chemical Society</i> , 2000, 122, 2903-2910.	6.6	38
71	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 18. Catalytic Transfer Dehydrogenation of Alkanes by an Iridium(III) Pincer Complex. <i>Organometallics</i> , 2001, 20, 2153-2160.	1.1	38
72	Generalized energy-based fragmentation approach for modeling condensed phase systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1297.	6.2	38

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73	Tetranuclear manganese(III) clusters containing both carboxylate and phosphonate bridging ligands. <i>Inorganica Chimica Acta</i> , 2007, 360, 1645-1650.	1.2	36
74	Structures and Spectroscopic Properties of Large Molecules and Condensed-Phase Systems Predicted by Generalized Energy-Based Fragmentation Approach. <i>Accounts of Chemical Research</i> , 2021, 54, 169-181.	7.6	36
75	Cooperativity in Long α - and 3×10^4 -Helical Polyalanines: Both Electrostatic and van der Waals Interactions Are Essential. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11462-11469.	1.2	35
76	The Generalized Energy-Based Fragmentation Approach with an Improved Fragmentation Scheme: Benchmark Results and Illustrative Applications. <i>ChemPhysChem</i> , 2013, 14, 108-115.	1.0	35
77	Homolytic Cleavage of a B-B Bond by the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification. <i>Angewandte Chemie</i> , 2016, 128, 6089-6093.	1.6	35
78	Electro-Descriptors for the Performance Prediction of Electro-Organic Synthesis. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 4199-4207.	7.2	35
79	Benchmark Relative Energies for Large Water Clusters with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2696-2704.	2.3	34
80	Enantioselective copper-catalysed defluorosilylation of trifluoro-methylated alkenes with silylboronates. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2618-2627.	2.3	34
81	Strength of Spin Coupling in High-Spin Organic Molecules. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5567-5573.	1.1	33
82	Mechanistic Insight on the Hydrogenation of Conjugated Alkenes with H ₂ Catalyzed by Early Main-Group Metal Catalysts. <i>Inorganic Chemistry</i> , 2010, 49, 3361-3369.	1.9	33
83	Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 756-766.	2.3	32
84	Fragmentation-Based QM/MM Simulations: Length Dependence of Chain Dynamics and Hydrogen Bonding of Polyethylene Oxide and Polyethylene in Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7061-7070.	1.2	31
85	Terahertz spectra of DNA nucleobase crystals: A joint experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 179, 255-260.	2.0	31
86	Theoretical Study toward Understanding the Catalytic Mechanism of Pyruvate Decarboxylase. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18664-18672.	1.2	30
87	Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for the Prediction of Activation Barriers, Spectroscopic Constants in Diatomic Molecules, and Singlet-Triplet Gaps in Diradicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12518-12525.	1.1	29
88	Is Ferromagnetic Spin Coupling Constant within Homologous Di- and Triradicals?. <i>The Journal of Physical Chemistry</i> , 1996, 100, 4775-4780.	2.9	28
89	A multireference configuration interaction method based on the separated electron pair wave functions. <i>Journal of Computational Chemistry</i> , 2006, 27, 39-47.	1.5	28
90	Generalized Energy-Based Fragmentation Approach for Localized Excited States of Large Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9667-9677.	1.1	28

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91	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5231-5239.	2.3	28
92	Density Functional Study on the Mechanisms of the Reactions of Gas-Phase OsOn+ (n = 1~4) with Methane. <i>Organometallics</i> , 2004, 23, 3656-3667.	1.1	27
93	New insight into selective catalytic reduction of nitrogen oxides by ammonia over H-form zeolites: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3304.	1.3	27
94	Energetics and Mechanism of Dinitrogen Cleavage at a Mononuclear Surface Tantalum Center: A New Way of Dinitrogen Reduction. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 8040-8043.	7.2	27
95	Block correlated coupled cluster method with the complete active-space self-consistent-field reference function: Applications for low-lying electronic excited states. <i>Journal of Chemical Physics</i> , 2009, 131, 174101.	1.2	27
96	Vibrational Spectra of Molecular Crystals with the Generalized Energy-Based Fragmentation Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2700-2711.	1.1	27
97	Selective Quadruple C(sp ³)-F Functionalization of Polyfluoroalkyl Ketones. <i>IScience</i> , 2020, 23, 101259.	1.9	27
98	Transition Metal Polyhydride Complexes. 11. Mechanistic Studies of the Cis to Trans Isomerization of the Iridium(III) Dihydride Ir(H) ₂ (CO)L (L = C ₆ H ₃ (CH ₂ P(H) ₂) ₂). <i>Organometallics</i> , 1999, 18, 5682-5687.	1.1	26
99	Refinement of DNA Structures through Near-Edge X-ray Absorption Fine Structure Analysis: Applications on Guanine and Cytosine Nucleobases, Nucleosides, and Nucleotides. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13214-13222.	1.2	25
100	Macrospirocyclic Oligomer Based on Triphenylamine and Diphenylphosphine Oxide as a Bipolar Host for Efficient Blue Electrophosphorescent Organic Light-Emitting Diodes (OLEDs). <i>Organic Letters</i> , 2015, 17, 1413-1416.	2.4	25
101	Spectroscopic Constants of Single-Bond Diatomic Molecules and Singlet~Triplet Gaps of Diradicals by the Block-Correlated Coupled Cluster Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4703-4709.	1.1	24
102	Understanding the Role of Intra- and Intermolecular Interactions in the Formation of Single- and Double-Helical Structures of Aromatic Oligoamides: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1335-1342.	1.1	24
103	Systematic Study of Soft X-ray Spectra of Poly(Dg)~Poly(Dc) and Poly(Da)~Poly(Dt) DNA Duplexes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7016-7021.	1.2	24
104	Fully optimized implementation of the cluster~molecule local correlation approach for electron correlation calculations of large systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 1130-1140.	1.5	24
105	Metal-free reductive coupling of aliphatic aldehydes/ketones with 4-cyanopyridines: expanded scope and mechanistic studies. <i>Organic Chemistry Frontiers</i> , 2020, 7, 2744-2751.	2.3	24
106	Pair-correlated coupled cluster theory: An alternative multireference coupled cluster method. <i>Journal of Chemical Physics</i> , 2003, 118, 5736-5745.	1.2	23
107	Insight into the reaction between a primary amine and a cavitand with an introverted aldehyde group: an enzyme-like mechanism. <i>Chemical Communications</i> , 2013, 49, 1542.	2.2	23
108	Charge-Transfer-Induced Selective sp ² C~H Bond Activation of Arenes by Use of a Hypervalent Iodine Compound: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2017, 82, 2984-2991.	1.7	23

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109	â€œInverseâ€Frustrated Lewis Pairs: An Inverse FLP Approach to the Catalytic Metal Free Hydrogenation of Ketones. <i>Chemistry - A European Journal</i> , 2018, 24, 16526-16531.	1.7	23
110	An On-the-Fly Approach to Construct Generalized Energy-Based Fragmentation Machine Learning Force Fields of Complex Systems. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5007-5014.	1.1	23
111	An MP2 study of linear polarizabilities and second-order hyperpolarizabilities for centrosymmetric squaraines. <i>Chemical Physics Letters</i> , 2002, 354, 316-323.	1.2	22
112	Fragment energy approach to Hartreeâ€Fock calculations of macromolecules. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2008, 104, 256.	4.4	22
113	Theoretical Study on the Mechanism of the Petasisâ€type Boronic Mannich Reaction of Organoboronic Acids, Amines, and α -Hydroxy Aldehydes. <i>Chinese Journal of Chemistry</i> , 2010, 28, 41-49.	2.6	22
114	A coupled cluster approach with a hybrid treatment of connected triple excitations for bond-breaking potential energy surfaces. <i>Journal of Chemical Physics</i> , 2010, 132, 114115.	1.2	22
115	Metal complexes formed by metal-assisted solvolysis of di-pyridylketone azine: structures and magnetic properties. <i>Dalton Transactions</i> , 2007, , 1838.	1.6	21
116	Theoretical study on the mechanism of H ₂ activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh. <i>Dalton Transactions</i> , 2010, 39, 857-863.	1.6	21
117	Circularly Polarized Luminescence of Chiral Perylene Diimide Based Enantiomers Triggered by Supramolecular Self-Assembly. <i>Chemistry - A European Journal</i> , 2016, 22, 12910-12915.	1.7	21
118	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5787-5796.	2.3	21
119	Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes. <i>Chemical Physics Letters</i> , 2012, 541, 7-11.	1.2	20
120	Mechanistic Insight on the Dielsâ€Alder Reaction Catalyzed by a Self-Assembled Molecular Capsule. <i>Journal of Organic Chemistry</i> , 2013, 78, 3577-3582.	1.7	20
121	Cluster-in-molecule local correlation method for large systems. <i>Science China Chemistry</i> , 2014, 57, 78-86.	4.2	20
122	Multireference Second Order Perturbation Theory with a Simplified Treatment of Dynamical Correlation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4634-4643.	2.3	20
123	Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16491-16500.	1.3	20
124	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4072-4081.	1.3	19
125	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 141-153.	2.3	19
126	Accurate and Efficient Prediction of NMR Parameters of Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2995-3005.	2.3	19

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127	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. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13547-13557.	1.3	18
128	Building quantum mechanics quality force fields of proteins with the generalized energy-based fragmentation approach and machine learning. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1326-1337.	1.3	18
129	Electron Correlation and Magnetism: A Simple Molecular Orbital Approach for Predicting Ground-State Spins of Conjugated Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5587-5592.	1.1	17
130	An efficient linear scaling procedure for constructing localized orbitals of large molecules based on the one-particle density matrix. <i>Journal of Chemical Physics</i> , 2011, 135, 134107.	1.2	17
131	Tuning Charge Balance in Solution-Processable Bipolar Triphenylamine-diazafluorene Host Materials for Phosphorescent Devices. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 9445-9452.	4.0	17
132	Accurate Relative Energies and Binding Energies of Large Ice-Liquid Water Clusters and Periodic Structures. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4030-4038.	1.1	17
133	Biofumigation with volatile organic compounds from <i>Streptomyces alboflavus</i> and pure chemicals to control <i>Aspergillus ochraceus</i> . <i>Annals of Applied Biology</i> , 2018, 173, 313-322.	1.3	17
134	Theoretical Study on the Diels-Alder Reaction between 2-Methylacrolein and Cyclopentadiene Catalyzed by a Cationic Oxazaborolidine Lewis Acid. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9225-9230.	1.1	16
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